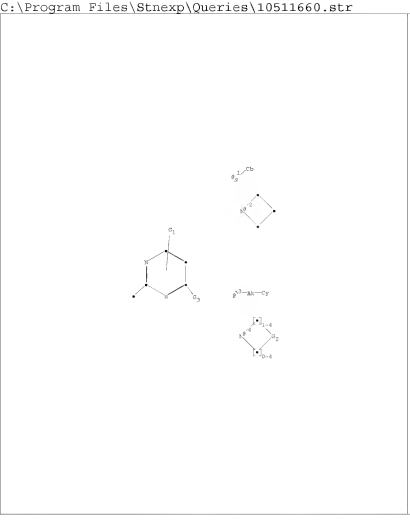
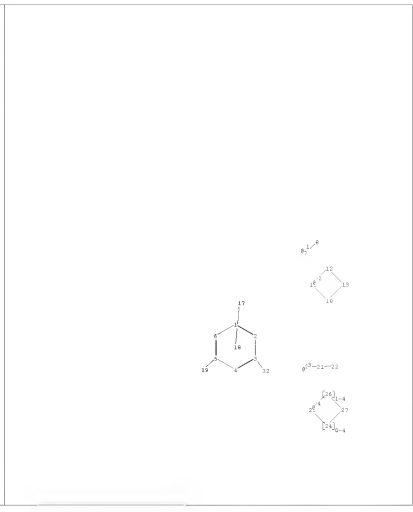
C:\Program Files\Stnexp\Queries\10511660.str





```
chain nodes :
    7  8  17  20  21  22  32
ring nodes :
    1  2  3  4  5  6  10  11  12  13  24  25  26  27
ring/chain nodes :
    19
chain bonds :
    3-32  5-19  7-8  20-21  21-22
ring bonds :
    1-2  1-6  2-3  3-4  4-5  5-6  10-11  10-13  11-12  12-13  24-25  24-27  25-26  26-27
exact/norm bonds :
    3-32  5-19  7-8  10-11  10-13  11-12  12-13  20-21  21-22  24-25  24-27  25-26  26-27
normalized bonds :
    1-2  1-6  2-3  3-4  4-5  5-6
isolated ring systems :
    containing 1 : 10 :

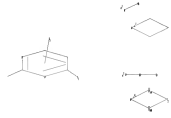

G1:[*1],[*2]

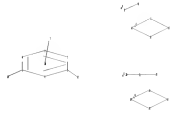
G2:C,S

G3:[*1],[*3],[*4]

Match level :
    1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:CLASS  8:Atom  10:Atom  11:Atom  12:Atom
    13:Atom  17:CLASS  18:Atom  19:CLASS  20:CLASS  21:CLASS  22:Atom  24:Atom  25:Atom  26:Atom
    27:Atom  32:CLASS
Generic attributes :
    8:
    Saturation             : Saturated
    22:
    Saturation             : Unsaturated
```

=>
Uploading C:\Program Files\Stnexp\Queries\10511660.str





chain nodes :
7 8 17 20 21 22 32
ring nodes :
1 2 3 4 5 6 10 11 12 13 24 25 26 27
ring/chain nodes :
19
chain bonds :
3-32 5-19 7-8 20-21 21-22
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-13 11-12 12-13 24-25 24-27 25-26
26-27
exact/norm bonds :

```
3-32  5-19  7-8  10-11  10-13  11-12  12-13  20-21  21-22  24-25  24-27  25-26
26-27
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6
isolated ring systems :
containing 1 : 10 :


G1:[*1],[*2]

G2:C,S

G3:[*1],[*3],[*4]

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:CLASS  8:Atom  10:Atom  11:Atom
12:Atom  13:Atom  17:CLASS  18:Atom  19:CLASS  20:CLASS  21:CLASS  22:Atom  24:Atom
 25:Atom  26:Atom  27:Atom  32:CLASS
Generic attributes :
8:
Saturation             : Saturated
22:
Saturation             : Unsaturated




L1      STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


=> s l1 sss sam
SAMPLE SEARCH INITIATED 15:31:50 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     5091 TO ITERATE

 39.3% PROCESSED     2000 ITERATIONS                                 2 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        97542 TO   106098
PROJECTED ANSWERS:               2 TO      236

L2            2 SEA SSS SAM L1

=> => s l1 sss ful
FULL SEARCH INITIATED 15:32:16 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   103018 TO ITERATE
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100.0% PROCESSED 103018 ITERATIONS 231 ANSWERS
SEARCH TIME: 00.00.01

L3 231 SEA SSS FUL L1

=> => s l3
L4 13 L3

=> d l4 1-13 bib,ab,hitstr

L4 ANSWER 1 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2008:191744 CAPLUS
DN 148:262855
TI Preparation of carbocyclic purine nucleoside analogs as antitumor agents and inhibitors of E1 activating enzymes
IN Claiborne, Christopher F.; Critchley, Stephen; Langston, Steven P.; Olhava, Edward J.; Peluso, Stephane; Weatherhead, Gabriel S.; Vyskocil, Stepan; Visiers, Irache; Mizutani, Hiro; Cullis, Courtney
PA Millennium Pharmaceuticals, Inc., USA
SO PCT Int. Appl., 204pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2008019124	A1	20080214	WO 2007-US17463	20070806
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW			
	RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	US 20080051404	A1	20080228	US 2007-890338	20070806
PRAI	US 2006-836158P	P	20060808		

OS MARPAT 148:262855
AB Nucleoside derivs. I, wherein A is 6-membered nitrogen-containing heteroaryl ring, optionally fused to a 5- or 6-membered aryl, heteroaryl, cyclo-aliphatic or heterocyclic ring; W is -CH-, -CHF-, -CF2-, -CH(R')-, -CF(R')-, -NH-, -N(R')-, -O-, -S-, or -NHC(O)-; R' is aliphatic, fluoro-aliph, alkylene chain that is attached to a ring position on ring A to form a 5-, 6-, or 7-membered fused ring, wherein the alkylene chain optionally is substituted with Cl, aliphatic, fluoro-aliphatic, O, -CN, or amide; X is CH2, CHF, CF2, NH, O; Y is O, S, substituted carbon; each R is independently H, F, aliphatic, fluoro-aliphatic; two R, taken together with the carbon atom to which they are attached, form a 3- to 6-membered carbocyclic ring; or one R, taken together with R1 and the intervening carbon atoms, forms a 3- to 6-membered spiro-cyclic ring; or two R together form O; R1 is H, or aliphatic; R and R1 taken together with the intervening carbon atoms form a 3- to 6-membered spiro-cyclic ring; R2 and R5 are independently is H , F , CN, N3, OH , alkoxy, substituted hydrazine, carbamate, amide, acyl, oxy-amide, ester, oxy-carboxylate, fluoro-aliphatic, aliphatic; R3 is H , F , aliphatic, fluoro-aliphatic; R4 is H, F, aliphatic, fluoro-aliphatic; R6 is H, aliphatic; n is 1-3; were prepared as inhibitors of E1 activating enzymes and useful for treating disorders, particularly cell proliferation disorders, including cancers, inflammatory and neurodegenerative disorders; and inflammation associated with infection and cachexia. Thus, carbocyclic nucleoside analog II was prepared and tested in vitro and in mice as inhibitor of E1 activating enzyme. The compds. are designed to be inhibitors of Nedd8-activating enzyme

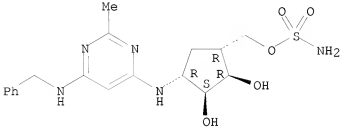
(APPBP1-Uba3) (NAE), ubiquitin activating enzyme (UAE), and/or activating enzyme (Aos1-Uba2) (SAE).

IT 1007123-74-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of carbocyclic purine nucleoside analogs as antitumor agents and inhibitors of E1 activating enzymes)

RN 1007123-74-1 CAPLUS

CN Sulfamic acid, [(1R,2R,3S,4R)-2,3-dihydroxy-4-[[2-methyl-6-[(phenylmethyl)amino]-4-pyrimidinyl]amino]cyclopentyl]methyl ester (CA INDEX NAME)

Absolute stereochemistry.

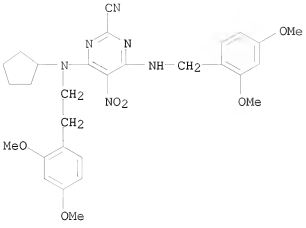


RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2007:1468933 CAPLUS
DN 148:100632
TI Preparation of pteridine derivatives as cathepsin inhibitors
IN Heald, Robert Andrew; Morley, Andrew David
PA Astrazeneca AB, Swed.; Astrazeneca UK Limited
SO PCT Int. Appl., 34pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

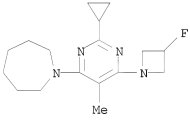
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2007148064	A1	20071227	WO 2007-GB2269	20070620
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW			
	RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
PRAI	US 2006-816157P	P	20060623		

OS MARPAT 148:100632
AB The title compds. I [X = NR1 or S; Y = O or NR4; X1 = a bond, NH or N(alkyl); R = 4-7 membered saturated monocyclic or bicyclic ring (optionally containing one or more O, S(O)0-2 or N atoms), etc.; R1 = (CH2)nY(CH2)pR7 (wherein n, p = 0-2; Y = a bond, O, SO0-2 or R8; R7 = 3-7 membered saturated ring optionally containing one or more O, S or N atoms, or aryl, heteroaryl, etc.; R8 = H, alkyl, cycloalkyl); R2, R3 = H or alkyl; R4 = H, alkyl, cycloalkyl], useful for treating diseases associated with cysteine protease activity, were prepared and formulated. E.g., a multi-step synthesis of II, starting from benzyloxyacetaldehyde and ethanolamine, was given. The compds. I are reversible inhibitors of cysteine proteases S, K, F, L and B. Of particular interest are diseases associated with Cathepsin K. Compds. I were screened in an assay for identification of cathepsin K inhibitors (no data given).
IT 1000186-18-4P
RL: PRPH (Prophetic); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pteridine derivs. as cathepsin inhibitors)
RN 1000186-18-4 CAPLUS
CN 2-Pyrimidinecarbonitrile, 4-[cyclopentyl[2-(2,4-dimethoxyphenyl)ethyl]amino]-6-[[(2,4-dimethoxyphenyl)methyl]amino]-5-nitro- (CA INDEX NAME)

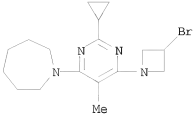


RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

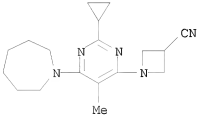
L4 ANSWER 3 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2007:526089 CAPLUS
DN 147:45200
TI Dual M3 antagonists-PDE4 inhibitors. Part 2: Synthesis and SAR of 3-substituted azetidinyl derivatives
AU Provins, Laurent; Christophe, Bernard; Danhaive, Pierre; Dulieu, Jacques; Gillard, Michel; Quere, Luc; Stebbins, Karin
CS R&D, Chemin du Foriest, UCB Pharma S.A., Braine-L'Alleud, B-1420, Belg.
SO Bioorganic & Medicinal Chemistry Letters (2007), 17(11), 3077-3080
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier Ltd.
DT Journal
LA English
OS CASREACT 147:45200
AB Introduction of 3-substituted azetidinyl substituents onto the 4,6-diaminopyrimidine scaffold allowed the improvement of PDE4 inhibiting activities. Preliminary in vivo activity in pulmonary inflammation models is reported.
IT 617719-14-9P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(Dual M3 antagonists-PDE4 inhibitors. Part 2: Synthesis and SAR of 3-substituted azetidinyl derivs.)
RN 617719-14-9 CAPLUS
CN 1H-Azepine, 1-[2-cyclopropyl-6-(3-fluoro-1-azetidinyl)-5-methyl-4-pyrimidinyl]hexahydro- (CA INDEX NAME)



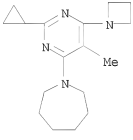
IT 617718-72-6P 617718-73-7P 617718-74-8P
617718-76-0P 617718-81-7P 617718-83-9P
617718-85-1P 617718-87-3P 617718-89-5P
617718-91-9P 790656-98-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(Dual M3 antagonists-PDE4 inhibitors. Part 2: Synthesis and SAR of 3-substituted azetidinyl derivs.)
RN 617718-72-6 CAPLUS
CN 1H-Azepine, 1-[6-(3-bromo-1-azetidinyl)-2-cyclopropyl-5-methyl-4-pyrimidinyl]hexahydro- (CA INDEX NAME)



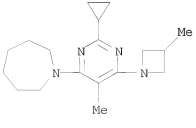
RN 617718-73-7 CAPLUS
CN 3-Azetidinecarbonitrile, 1-[2-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl-4-pyrimidinyl]- (CA INDEX NAME)



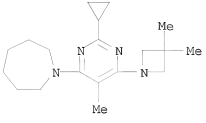
RN 617718-74-8 CAPLUS
CN 1H-Azepine, 1-[6-(1-azetidinyl)-2-cyclopropyl-5-methyl-4-pyrimidinyl]hexahydro- (CA INDEX NAME)



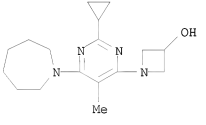
RN 617718-76-0 CAPLUS
CN 1H-Azepine, 1-[2-cyclopropyl-5-methyl-6-(3-methyl-1-azetidinyl)-4-pyrimidinyl]hexahydro- (CA INDEX NAME)



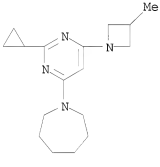
RN 617718-81-7 CAPLUS
CN 1H-Azepine, 1-[2-cyclopropyl-6-(3,3-dimethyl-1-azetidinyl)-5-methyl-4-pyrimidinyl]hexahydro- (CA INDEX NAME)



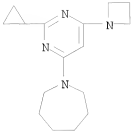
RN 617718-83-9 CAPLUS
CN 3-Azetidinol, 1-[2-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl-4-pyrimidinyl]- (CA INDEX NAME)



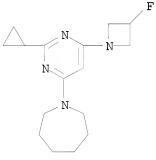
RN 617718-85-1 CAPLUS
CN 1H-Azepine, 1-[2-cyclopropyl-6-(3-methyl-1-azetidinyl)-4-pyrimidinyl]hexahydro- (CA INDEX NAME)



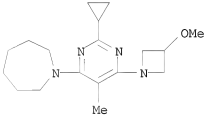
RN 617718-87-3 CAPLUS
CN 1H-Azepine, 1-[6-(1-azetidinyl)-2-cyclopropyl-4-pyrimidinyl]hexahydro- (CA INDEX NAME)



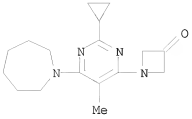
RN 617718-89-5 CAPLUS
CN 1H-Azepine, 1-[2-cyclopropyl-6-(3-fluoro-1-azetidinyl)-4-pyrimidinyl]hexahydro- (CA INDEX NAME)



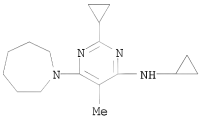
RN 617718-91-9 CAPLUS
CN 1H-Azepine, 1-[2-cyclopropyl-6-(3-methoxy-1-azetidinyl)-5-methyl-4-pyrimidinyl]hexahydro- (CA INDEX NAME)



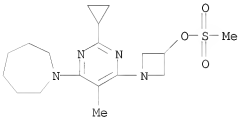
RN 790656-98-3 CAPLUS
CN 3-Azetidinone, 1-[2-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl-4-pyrimidinyl]- (CA INDEX NAME)



IT 617716-93-5, UCB 101333-3
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(Dual M3 antagonists-PDE4 inhibitors. Part 2: Synthesis and SAR of 3-substituted azetidinyl derivs.)
RN 617716-93-5 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl- (CA INDEX NAME)



IT 617718-84-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(Dual M3 antagonists-PDE4 inhibitors. Part 2: Synthesis and SAR of 3-substituted azetidinyl derivs.)
RN 617718-84-0 CAPLUS
CN 3-Azetidinol, 1-[2-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl-4-pyrimidinyl]-, 3-methanesulfonate (CA INDEX NAME)



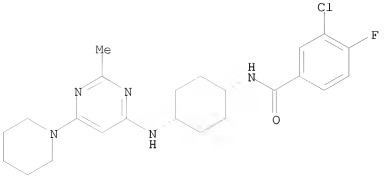
RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2007:405311 CAPLUS
DN 146:402000
TI Preparation of pyrimidine derivatives as MCH receptor antagonists
IN Sekiguchi, Yoshiisa; Kanuma, Yukihiro; Omodera, Katsunori; Tran, Thuy-Ahn; Semple, Graeme; Kramer, Bryan A.
PA Taisho Pharmaceutical Co., Ltd., Japan; Arena Pharmaceutical Inc.
SO Jpn. Kokai Tokkyo Koho, 187pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 2007091649	A	20070412	JP 2005-284040	20050929
PRAI JP 2005-284040		20050929		

OS MARPAT 146:402000
AB Title compds. Q-L-Y-R1 [I; Q = Q1, etc.; R1 = alkyl, alkenyl, alkynyl, etc.; R2 = halo, alkyl, halo-substituted alkyl, etc.; L = Q2, Q3, etc.; R3, R4 = H, alkyl; A, B = single bond, -CH2-, -(CH2)2-; Z1, Z2 = H, halo, alkyl, etc.; R2 and Z2 may combine to form a cycle, -R2-Z2- is -(CH2)n- or -(CH2)O-CH:CH-(CH2)p- (one -CH2- in -R2-Z2- may be replaced with C(O), O, S, etc.); n = 2-6; o, p = 0-4 such as o + p = 0-4; when L is Q2, etc., Y is -C(O)O-, -S(O)2-, -C(O)-, etc.; when L is Q3, etc., Y is -C(O)NR5, -C(S)NR5, -C(O)O-, etc.; R5 = H, alkyl], pharmaceutically acceptable salts, hydrates, or solvates thereof were prepared For example, reaction of N-(cis-4-aminocyclohexyl)-2,N',N'-trimethylpyrimidine-4,6-diamine, e.g., prepared from (cis-4-aminocyclohexyl)carbamic acid tert-Bu ester in 4 steps, with 4-fluorobenzoyl chloride followed by treatment with HCl afforded compound II hydrochloride [R = F; R' = H]. In melanin concentrating hormone (MCH) antagonistic assays, the IC50 value of compound II hydrochloride [R = H; R' = Cl] was 26 nM. Compds. I are claimed useful for the treatment of anxiety, depression, etc.
IT 866643-12-1P, 3-Chloro-4-fluoro-N-[cis-4-[(2-methyl-6-(piperidin-1-yl)pyrimidin-4-yl)amino]cyclohexyl]benzamide hydrochloride
866643-15-4P, 3-Chloro-4-fluoro-N-[cis-4-[(2-methyl-6-(pyrrolidin-1-yl)pyrimidin-4-yl)amino]cyclohexyl]benzamide hydrochloride
866644-74-8P, N-(cis-4-[[6-(Cyclopropylamino)-2-methylpyrimidin-4-yl]amino]cyclohexyl)-3,4,5-trifluorobenzamide hydrochloride
866644-76-0P, N-[cis-4-([6-[Benzyl(methyl)amino]-2-methylpyrimidin-4-yl]amino)cyclohexyl]-3,4,5-trifluorobenzamide hydrochloride
866648-27-3P, 3-Chloro-4-fluoro-N-cis-4-[(2-methyl-6-piperidin-1-ylpyrimidin-4-yl)amino]cyclohexylbenzamide 866648-34-2P, 3-Chloro-4-fluoro-N-cis-4-[(2-methyl-6-pyrrolidin-1-ylpyrimidin-4-yl)amino]cyclohexylbenzamide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of pyrimidine derivs. as MCH receptor antagonists for treatment of anxiety and depression)
RN 866643-12-1 CAPLUS
CN Benzamide, 3-chloro-4-fluoro-N-[cis-4-[[2-methyl-6-(1-piperidinyl)-4-pyrimidinyl]amino]cyclohexyl]-, hydrochloride (1:1) (CA INDEX NAME)

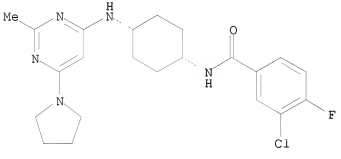
Relative stereochemistry.



● HCl

RN 866643-15-4 CAPLUS
CN Benzamide, 3-chloro-4-fluoro-N-[cis-4-[[2-methyl-6-(1-pyrrolidinyl)-4-pyrimidinyl]amino]cyclohexyl]-, hydrochloride (1:1) (CA INDEX NAME)

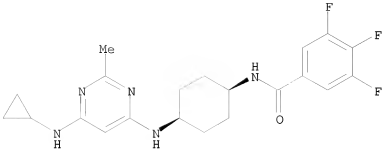
Relative stereochemistry.



● HCl

RN 866644-74-8 CAPLUS
CN Benzamide, N-[cis-4-[[6-(cyclopropylamino)-2-methyl-4-pyrimidinyl]amino]cyclohexyl]-3,4,5-trifluoro-, hydrochloride (1:1) (CA INDEX NAME)

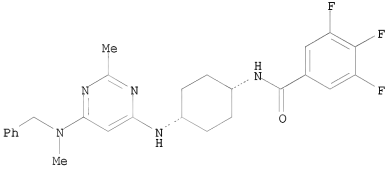
Relative stereochemistry.



● HCl

RN 866644-76-0 CAPLUS
CN Benzamide, 3,4,5-trifluoro-N-[cis-4-[[2-methyl-6-[methyl(phenylmethyl)amino]-4-pyrimidinyl]amino]cyclohexyl]-, hydrochloride (1:1) (CA INDEX NAME)

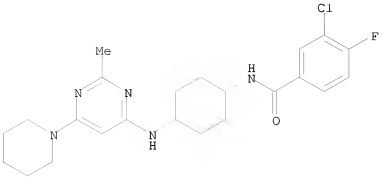
Relative stereochemistry.



● HCl

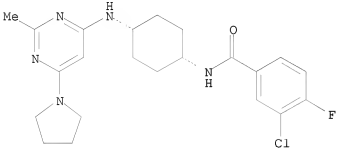
RN 866648-27-3 CAPLUS
CN Benzamide, 3-chloro-4-fluoro-N-[cis-4-[[2-methyl-6-(1-piperidinyl)-4-pyrimidinyl]amino]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



RN 866648-34-2 CAPLUS
CN Benzamide, 3-chloro-4-fluoro-N-[cis-4-[[2-methyl-6-(1-pyrrolidinyl)-4-pyrimidinyl]amino]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.

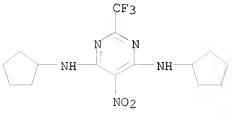


L4 ANSWER 5 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2006:1356771 CAPLUS
DN 146:100715
TI Preparation of pyrimidine derivatives for the treatment of gaba b mediated nervous system disorders
IN Floersheim, Philipp; Froestl, Wolfgang; Guery, Sebastien; Kaupmann, Klemens; Koller, Manuel
PA Novartis AG, Switz.; Novartis Pharma GmbH
SO PCT Int. Appl., 114pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2006136442	A1	20061228	WO 2006-EP6083	20060623
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW			
	RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	AU 2006261122	A1	20061228	AU 2006-261122	20060623
	CA 2610742	A1	20061228	CA 2006-2610742	20060623
	EP 1896428	A1	20080312	EP 2006-762168	20060623
	R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR				
	IN 2007DN09085	A	20080104	IN 2007-DN9085	20071126
	CN 101193868	A	20080604	CN 2006-80020794	20071211
	MX 200716395	A	20080307	MX 2007-16395	20071218
	KR 2008017382	A	20080226	KR 2007-729918	20071221
PRAI	GB 2005-12844	A	20050623		
	WO 2006-EP6083	W	20060623		

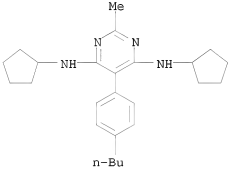
OS MARPAT 146:100715
AB Title compds. I in free base form or in acid addition salt form, in which R1 is an alkyl, haloalkyl, alkoxy, haloalkoxy, alkylthio, etc.; R2 is H, halo, substituted amino etc.; R3 is a halo, haloalkyl, nitro (un)substituted aryl or (un)substituted heteroaryl; R4 is a H, halo, hydroxyl, alkynyl, (un)substituted amino etc.; and A is a bond, alkandiyl, alkendiyl or alkyndiyl group are prepared as medicaments for the treatment of certain nervous system disorders and to medicaments comprising them. Thus, II was prepared and showed an inhibition of 77% at 1 μM of GABA and 2.5 μM of II.
IT 917895-56-8P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of pyrimidine derivs. for the treatment of gaba b mediated nervous system disorders)
RN 917895-56-8 CAPLUS
CN 4,6-Pyrimidinediamine, N4,N6-dicyclopentyl-5-nitro-2-(trifluoromethyl)-

(CA INDEX NAME)

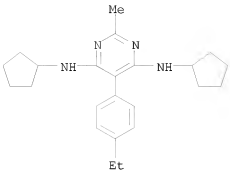


IT 917895-80-8P 917895-81-9P 917895-82-0P
917895-83-1P 917895-84-2P 917895-85-3P
917896-53-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrimidine derivs. for the treatment of gaba b mediated nervous system disorders)

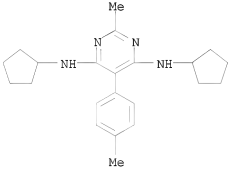
RN 917895-80-8 CAPLUS
CN 4,6-Pyrimidinediamine, 5-(4-butylphenyl)-N4,N6-dicyclopentyl-2-methyl-
(CA INDEX NAME)



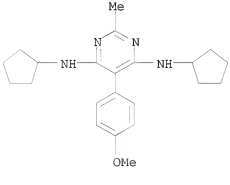
RN 917895-81-9 CAPLUS
CN 4,6-Pyrimidinediamine, N4,N6-dicyclopentyl-5-(4-ethylphenyl)-2-methyl-
(CA INDEX NAME)



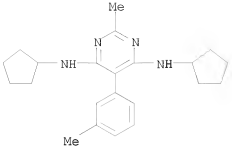
RN 917895-82-0 CAPLUS
CN 4,6-Pyrimidinediamine, N4,N6-dicyclopentyl-2-methyl-5-(4-methylphenyl)-
(CA INDEX NAME)



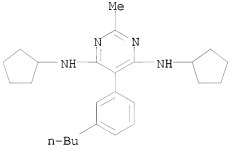
RN 917895-83-1 CAPLUS
CN 4,6-Pyrimidinediamine, N4,N6-dicyclopentyl-5-(4-methoxyphenyl)-2-methyl-
(CA INDEX NAME)



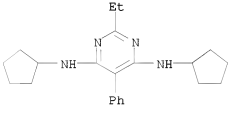
RN 917895-84-2 CAPLUS
CN 4,6-Pyrimidinediamine, N4,N6-dicyclopentyl-2-methyl-5-(3-methylphenyl)-
(CA INDEX NAME)



RN 917895-85-3 CAPLUS
CN 4,6-Pyrimidinediamine, 5-(3-butylphenyl)-N4,N6-dicyclopentyl-2-methyl- (CA INDEX NAME)



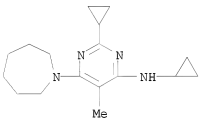
RN 917896-53-8 CAPLUS
CN 4,6-Pyrimidinediamine, N4,N6-dicyclopentyl-2-ethyl-5-phenyl- (CA INDEX NAME)



RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2006:188875 CAPLUS
DN 144:432767
TI First dual M3 antagonists-PDE4 inhibitors: Synthesis and SAR of 4,6-diaminopyrimidine derivatives
AU Provins, Laurent; Christophe, Bernard; Danhaive, Pierre; Dulieu, Jacques; Durieu, Veronique; Gillard, Michel; Lebon, Florence; Lengele, Sebastien; Quere, Luc; van Keulen, BerendJan
CS Global Chemistry, UCB, R&D, Chemin du Foriest, Braine-L'Alleud, B-1420, Belg.
SO Bioorganic & Medicinal Chemistry Letters (2006), 16(7), 1834-1839
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier B.V.
DT Journal
LA English
OS CASREACT 144:432767
AB Structure-activity studies around 4,6-diaminopyrimidine derivs. allowed the discovery of potent dual M3 antagonists and PDE4 inhibitors. Various chemical modulations around that scaffold led to the discovery of ucb-101333-3 (I) which is characterized by the most interesting profile on both targets.
IT 617716-93-5P
RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of 4,6-diaminopyrimidine derivs. as dual M3 antagonists and PDE4 inhibitors)
RN 617716-93-5 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl- (CA INDEX NAME)

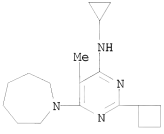
common inventors



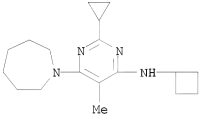
IT 617716-90-2P 617716-98-0P 617717-02-9P
617717-04-1P 617717-05-2P 617717-06-3P
617717-07-4P 617717-13-2P 617717-14-3P
617717-15-4P 617717-19-8P 617717-27-8P
617717-28-9P 617717-30-3P 617717-33-6P
617717-39-2P 617717-43-8P 617717-46-1P
617717-50-7P 617717-68-7P 617717-72-3P
617717-74-5P 617717-78-9P 617717-84-7P
617717-87-0P 617717-89-2P 617717-96-1P
617717-98-3P 617718-03-3P 617718-12-4P
617718-20-4P 617718-29-3P 617718-56-6P
617718-61-3P 617718-69-1P 617718-93-1P
762238-39-1P 765268-74-4P 773846-88-1P
792904-99-5P 884842-63-1P 884842-64-2P
884842-65-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL

(Biological study); PREP (Preparation)
(preparation of 4,6-diaminopyrimidine derivs. as dual M3 antagonists and PDE4 inhibitors)

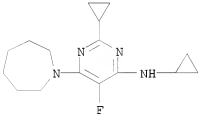
RN 617716-90-2 CAPLUS
CN 4-Pyrimidinamine, 2-cyclobutyl-N-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl- (CA INDEX NAME)



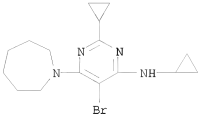
RN 617716-98-0 CAPLUS
CN 4-Pyrimidinamine, N-cyclobutyl-2-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl- (CA INDEX NAME)



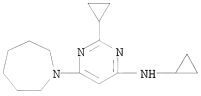
RN 617717-02-9 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-5-fluoro-6-(hexahydro-1H-azepin-1-yl)-(CA INDEX NAME)



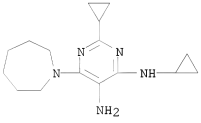
RN 617717-04-1 CAPLUS
CN 4-Pyrimidinamine, 5-bromo-N,2-dicyclopropyl-6-(hexahydro-1H-azepin-1-yl)-(CA INDEX NAME)



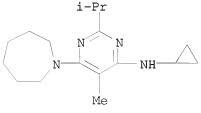
RN 617717-05-2 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-6-(hexahydro-1H-azepin-1-yl)- (CA INDEX NAME)



RN 617717-06-3 CAPLUS
CN 4,5-Pyrimidinediamine, N4,2-dicyclopropyl-6-(hexahydro-1H-azepin-1-yl)- (CA INDEX NAME)



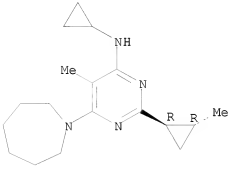
RN 617717-07-4 CAPLUS
CN 4-Pyrimidinamine, N-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl-2-(1-methylethyl)- (CA INDEX NAME)



RN 617717-13-2 CAPLUS
CN 4-Pyrimidinamine, N-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl-2-

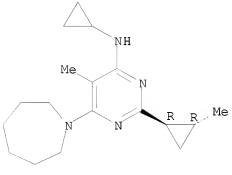
[(1R,2R)-2-methylcyclopropyl]-, rel-(-)- (CA INDEX NAME)

Rotation (-). Absolute stereochemistry unknown.

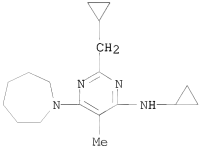


RN 617717-14-3 CAPLUS
CN 4-Pyrimidinamine, N-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl-2-[(1R,2R)-2-methylcyclopropyl]-, rel-(+)- (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.

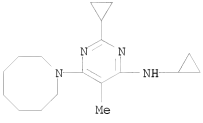


RN 617717-15-4 CAPLUS
CN 4-Pyrimidinamine, N-cyclopropyl-2-(cyclopropylmethyl)-6-(hexahydro-1H-azepin-1-yl)-5-methyl- (CA INDEX NAME)



RN 617717-19-8 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-6-(hexahydro-1(2H)-azocinyl)-5-methyl-

(CA INDEX NAME)



RN 617717-27-8 CAPLUS
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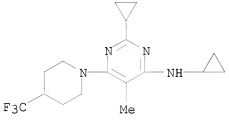
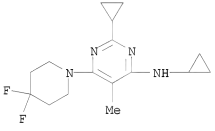
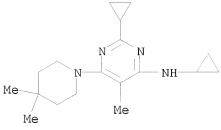


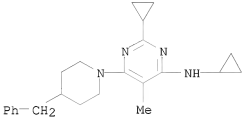
RN 617717-28-9 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-6-(4,4-difluoro-1-piperidinyl)-5-methyl- (CA INDEX NAME)



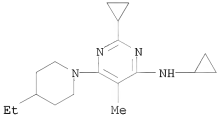
RN 617717-30-3 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-6-(4,4-dimethyl-1-piperidinyl)-5-methyl- (CA INDEX NAME)



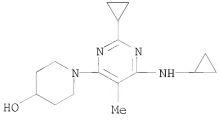
RN 617717-33-6 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-5-methyl-6-[4-(phenylmethyl)-1-piperidinyl]- (CA INDEX NAME)



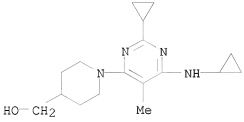
RN 617717-39-2 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-6-(4-ethyl-1-piperidinyl)-5-methyl- (CA INDEX NAME)



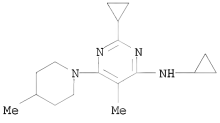
RN 617717-43-8 CAPLUS
CN 4-Piperidinol, 1-[2-cyclopropyl-6-(cyclopropylamino)-5-methyl-4-pyrimidinyl]- (CA INDEX NAME)



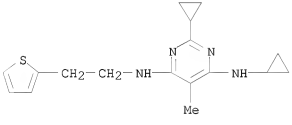
RN 617717-46-1 CAPLUS
CN 4-Piperidinemethanol, 1-[2-cyclopropyl-6-(cyclopropylamino)-5-methyl-4-pyrimidinyl]- (CA INDEX NAME)



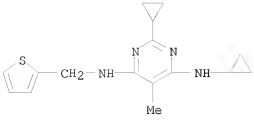
RN 617717-50-7 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-5-methyl-6-(4-methyl-1-piperidinyl)- (CA INDEX NAME)



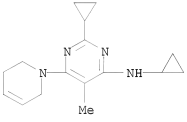
RN 617717-68-7 CAPLUS
CN 4,6-Pyrimidinediamine, N4,2-dicyclopropyl-5-methyl-N6-[2-(2-thienyl)ethyl]- (CA INDEX NAME)



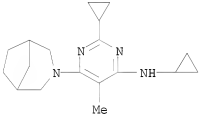
RN 617717-72-3 CAPLUS
CN 4,6-Pyrimidinediamine, N4,2-dicyclopropyl-5-methyl-N6-(2-thienylmethyl)- (CA INDEX NAME)



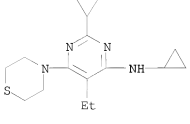
RN 617717-74-5 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-6-(3,6-dihydro-1(2H)-pyridinyl)-5-methyl- (CA INDEX NAME)



RN 617717-78-9 CAPLUS
CN 4-Pyrimidinamine, 6-(3-azabicyclo[3.2.1]oct-3-yl)-N,2-dicyclopropyl-5-methyl- (CA INDEX NAME)

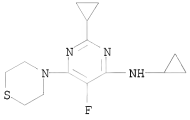


RN 617717-84-7 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-5-ethyl-6-(4-thiomorpholinyl)- (CA INDEX NAME)

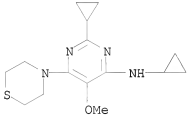


RN 617717-87-0 CAPLUS

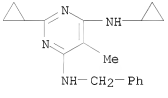
CN 4-Pyrimidinamine, N,2-dicyclopropyl-5-fluoro-6-(4-thiomorpholinyl)- (CA INDEX NAME)



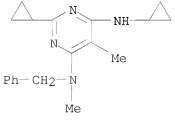
RN 617717-89-2 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-5-methoxy-6-(4-thiomorpholinyl)- (CA INDEX NAME)



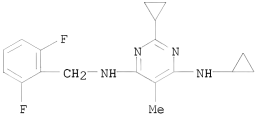
RN 617717-96-1 CAPLUS
CN 4,6-Pyrimidinediamine, N4,2-dicyclopropyl-5-methyl-N6-(phenylmethyl)- (CA INDEX NAME)



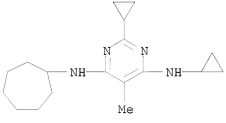
RN 617717-98-3 CAPLUS
CN 4,6-Pyrimidinediamine, N6,2-dicyclopropyl-N4,5-dimethyl-N4-(phenylmethyl)- (CA INDEX NAME)



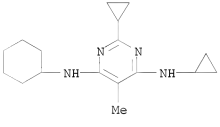
RN 617718-03-3 CAPLUS
CN 4,6-Pyrimidinediamine, N4,2-dicyclopropyl-N6-[(2,6-difluorophenyl)methyl]-5-methyl- (CA INDEX NAME)



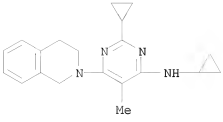
RN 617718-12-4 CAPLUS
CN 4,6-Pyrimidinediamine, N4-cycloheptyl-N6,2-dicyclopropyl-5-methyl- (CA INDEX NAME)



RN 617718-20-4 CAPLUS
CN 4,6-Pyrimidinediamine, N4-cyclohexyl-N6,2-dicyclopropyl-5-methyl- (CA INDEX NAME)

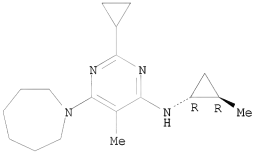


RN 617718-29-3 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-6-(3,4-dihydro-2(1H)-isoquinolinyl)-5-methyl- (CA INDEX NAME)

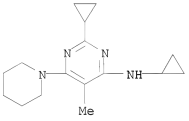


RN 617718-56-6 CAPLUS
CN 4-Pyrimidinamine, 2-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl-N-[(1R,2R)-2-methylcyclopropyl]-, rel- (CA INDEX NAME)

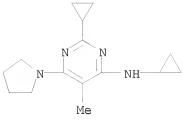
Relative stereochemistry.



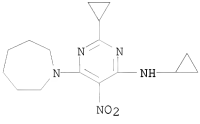
RN 617718-61-3 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-5-methyl-6-(1-piperidinyl)- (CA INDEX NAME)



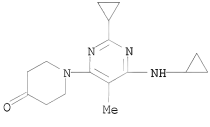
RN 617718-69-1 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-5-methyl-6-(1-pyrrolidinyl)- (CA INDEX NAME)



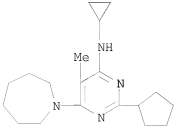
RN 617718-93-1 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-nitro- (CA INDEX NAME)



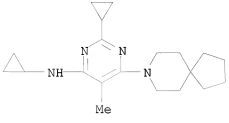
RN 762238-39-1 CAPLUS
CN 4-Piperidinone, 1-[2-cyclopropyl-6-(cyclopropylamino)-5-methyl-4-pyrimidinyl]- (CA INDEX NAME)



RN 765268-74-4 CAPLUS
CN 4-Pyrimidinamine, 2-cyclopentyl-N-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl- (CA INDEX NAME)



RN 773846-88-1 CAPLUS
CN 4-Pyrimidinamine, 6-(8-azaspiro[4.5]dec-8-yl)-N,2-dicyclopropyl-5-methyl- (CA INDEX NAME)



RN 792904-99-5 CAPLUS
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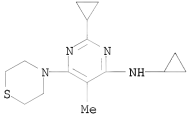
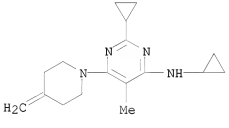


RN 884842-63-1 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-5-methyl-6-(4-methylene-1-piperidinyl)- (CA INDEX NAME)



RN 884842-64-2 CAPLUS
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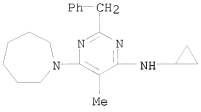

RN 884842-65-3 CAPLUS
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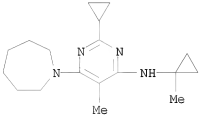

RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2005:1103757 CAPLUS
DN 143:387051
TI Preparation of pyrimidine derivatives as MCH antagonists for treatment of CNS disorders
IN Sekiguchi, Yoshinori; Kanuma, Kosuke; Omodera, Katsunori; Tran, Thuy-Anh; Semple, Graeme; Kramer, Bryan A.
PA Taisho Pharmaceutical Co., Ltd., Japan; Arena Pharmaceuticals, Inc
SO PCT Int. Appl., 281 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005095357	A2	20051013	WO 2005-JP6582	20050329
	WO 2005095357	A3	20060119		
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	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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	CA 2558915	A1	20051013	CA 2005-2558915	20050329
	EP 1730122	A2	20061213	EP 2005-721721	20050329
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	CN 1976905	A	20070606	CN 2005-80017519	20050329
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	JP 2007530445	T	20071101	JP 2006-534511	20050329
	IN 2006KN02816	A	20070601	IN 2006-KN2816	20060927
	MX 2006PA11198	A	20061211	MX 2006-PA11198	20060928
	KR 2007013279	A	20070130	KR 2006-720312	20060929
	NO 2006004950	A	20061229	NO 2006-4950	20061030
PRAI	US 2004-557406P	P	20040330		
	WO 2005-JP6582	W	20050329		

OS MARPAT 143:387051
AB Title compds. I, and II [wherein R1 = (un)substituted alk(en/yn)yl, cycloalk(en)yl, carbocyclyl, carbocyclic aryl, heterocyclyl; R2 = halo, (un)substituted alkyl, heterocyclyl, etc.; L = cyclohexylene-1,4-diamino, cyclohexylene-1-amino-4-aminomethylene, etc.; Z1-Z4 = independently H, halo, (un)substituted alkyl, etc.; Y = CONH and derivs., CO, SO, SO2, etc.; and pharmaceutically acceptable salts, hydrates, or solvates] were prepared as antagonists of melanin concentrating hormone (MCH), an endogenous ligand of G-protein coupled receptors (GPCRs). I were assayed using high throughput functional screening to detect intracellular Ca2+ concns. for accessing GPCR activation. For example, III•HCl was prepared by acylation N-(cis-4-aminocyclohexyl)-2-methyl-N',N'-dimethylpyrimidine-4,6-diamine (preparation given) with 4-fluorobenzoyl chloride, and acidulation of the free base (not isolated). The latter demonstrated MCH antagonist

activity with an IC50 value of 101 nM. Thus, pharmaceutical compns. comprising I are useful for the prophylaxis or treatment of improving memory function, sleeping and arousal, anxiety, depression, mood disorders, seizure, obesity, diabetes, appetite and eating disorders, cardiovascular disease, hypertension, dyslipidemia, myocardial infarction, binge eating disorders including bulimia, anorexia, mental disorders including manic depression, schizophrenia, delirium, dementia, stress, cognitive disorders, attention deficit disorder, substance abuse disorders, and dyskinesias including Parkinson's disease, epilepsy, and addiction (no data).

IT 866643-12-1P, 3-Chloro-4-fluoro-N-[cis-4-[[2-methyl-6-(piperidin-1-yl)pyrimidin-4-yl]amino]cyclohexyl]benzamide monohydrochloride
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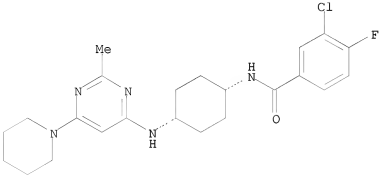
866648-27-3P, 3-Chloro-4-fluoro-N-[cis-4-[[2-methyl-6-(piperidin-1-yl)pyrimidin-4-yl]amino]cyclohexyl]benzamide 866648-34-2P, 3-Chloro-4-fluoro-N-[cis-4-[[2-methyl-6-(pyrrolidin-1-yl)pyrimidin-4-yl]amino]cyclohexyl]benzamide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of pyrimidines as MCH antagonists for treatment of CNS disorders)

RN 866643-12-1 CAPLUS

CN Benzamide, 3-chloro-4-fluoro-N-[cis-4-[[2-methyl-6-(1-piperidinyl)-4-pyrimidinyl]amino]cyclohexyl]-, hydrochloride (1:1) (CA INDEX NAME)

Relative stereochemistry.

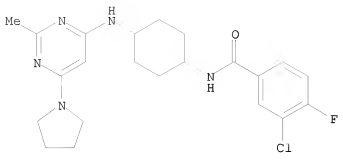


● HCl

RN 866643-15-4 CAPLUS

CN Benzamide, 3-chloro-4-fluoro-N-[cis-4-[[2-methyl-6-(1-pyrrolidinyl)-4-pyrimidinyl]amino]cyclohexyl]-, hydrochloride (1:1) (CA INDEX NAME)

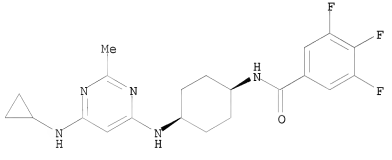
Relative stereochemistry.



● HCl

RN 866644-74-8 CAPLUS
CN Benzamide, N-[cis-4-[[6-(cyclopropylamino)-2-methyl-4-pyrimidinyl]amino]cyclohexyl]-3,4,5-trifluoro-, hydrochloride (1:1) (CA INDEX NAME)

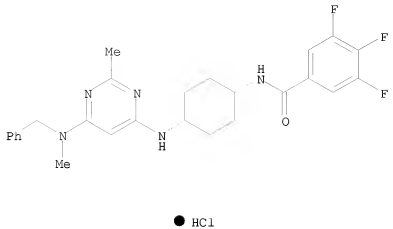
Relative stereochemistry.



● HCl

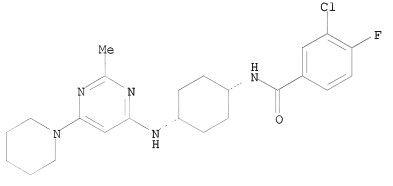
RN 866644-76-0 CAPLUS
CN Benzamide, 3,4,5-trifluoro-N-[cis-4-[[2-methyl-6-[methyl(phenylmethyl)amino]-4-pyrimidinyl]amino]cyclohexyl]-, hydrochloride (1:1) (CA INDEX NAME)

Relative stereochemistry.



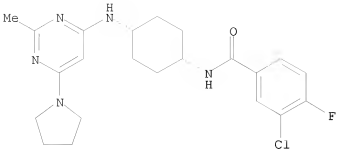
RN 866648-27-3 CAPLUS
CN Benzamide, 3-chloro-4-fluoro-N-[cis-4-[[2-methyl-6-(1-piperidinyl)-4-pyrimidinyl]amino]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



RN 866648-34-2 CAPLUS
CN Benzamide, 3-chloro-4-fluoro-N-[cis-4-[[2-methyl-6-(1-pyrrolidinyl)-4-pyrimidinyl]amino]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.


Me
N
N
H
N
N
O
N
H
F
Cl

L4 ANSWER 8 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2003:837052 CAPLUS
DN 139:337980
TI Preparation of aminopyrimidines with muscarinic M3 antagonist and PDE IV inhibiting activity
IN Provins, Laurent; Van Keulen, Berend Jan; Surtees, John; Talaga, Patrice; Christophe, Bernard
PA UCB, S.A., Belg.
SO PCT Int. Appl., 71 pp.
CODEN: PIXXD2
Applicant's
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003087064	A1	20031023	WO 2003-EP3299	20030329
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
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	AU 2003222786	A1	20031027	AU 2003-222786	20030329
	EP 1499598	A1	20050126	EP 2003-718717	20030329
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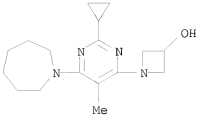
	US 20060074068	A1	20060406	US 2005-511660	20051005
PRAI	EP 2002-8706	A	20020418		
	WO 2003-EP3299	W	20030329		

OS MARPAT 139:337980
AB Aminopyrimidines I [R = NHR2, (un)substituted azetidinyl; R1 = alkyl, cycloalkyl; R2 = cycloalkyl; R3 = H, alkyl, halogen, OH, alkoxy, amino; R2R3 = alkylene; R4 = H, alkyl; R5 = cycloalkyl, aralkyl, heterocyclylalkyl; NR4R5 = heterocyclic], combining affinity and antagonism against the human M3 muscarinic receptor with activity as selective phosphodiesterase IV (PDE IV) inhibitors, were prepared Thus, the amine II was prepared from 6-chloro-N,2-dicyclopropyl-5-nitropyrimidin-4-amine by reaction with hexamethylenimine and reduction of the nitro group.
IT 617718-83-9P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of aminopyrimidines with muscarinic M3 antagonist and PDE IV inhibiting activity)
RN 617718-83-9 CAPLUS
CN 3-Azetidinol, 1-[2-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl-4-pyrimidinyl]- (CA INDEX NAME)



IT 617716-91-3P 617716-94-6P 617716-96-8P
617717-01-8P 617717-03-0P 617717-04-1P
617717-05-2P 617717-06-3P 617717-08-5P
617717-10-9P 617717-12-1P 617717-13-2P
617717-20-1P 617717-27-8P 617717-29-0P
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617717-40-5P 617717-49-4P 617717-51-8P
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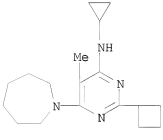
617718-04-4P 617718-25-9P 617718-27-1P
617718-39-5P 617718-62-4P 617718-64-6P
617718-66-8P 617718-69-1P 617718-75-9P
617718-76-0P 617718-77-1P 617718-79-3P
617718-86-2P 617718-87-3P 617718-89-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of aminopyrimidines with muscarinic M3 antagonist and PDE IV inhibiting activity)

RN 617716-91-3 CAPLUS

CN 4-Pyrimidinamine, 2-cyclobutyl-N-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl-, (2Z)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

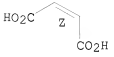
CRN 617716-90-2
CMF C18 H28 N4



CM 2

CRN 110-16-7
CMF C4 H4 O4

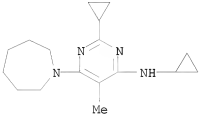
Double bond geometry as shown.



RN 617716-94-6 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl-, (2Z)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

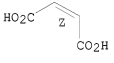
CRN 617716-93-5
CMF C17 H26 N4



CM 2

CRN 110-16-7
CMF C4 H4 O4

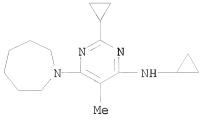
Double bond geometry as shown.



RN 617716-96-8 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl-, (2E)-2-butenedioate (2:3) (CA INDEX NAME)

CM 1

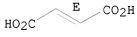
CRN 617716-93-5
CMF C17 H26 N4



CM 2

CRN 110-17-8
CMF C4 H4 O4

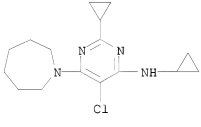
Double bond geometry as shown.



RN 617717-01-8 CAPLUS
CN 4-Pyrimidinamine, 5-chloro-N,2-dicyclopropyl-6-(hexahydro-1H-azepin-1-yl)-, (2Z)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

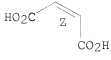
CRN 617717-00-7
CMF C16 H23 Cl N4



CM 2

CRN 110-16-7
CMF C4 H4 O4

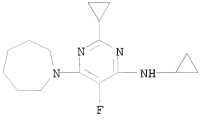
Double bond geometry as shown.



RN 617717-03-0 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-5-fluoro-6-(hexahydro-1H-azepin-1-yl)-, (2Z)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

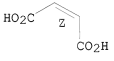
CRN 617717-02-9
CMF C16 H23 F N4



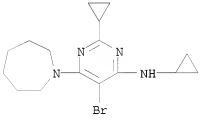
CM 2

CRN 110-16-7
CMF C4 H4 O4

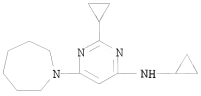
Double bond geometry as shown.



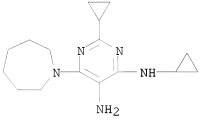
RN 617717-04-1 CAPLUS
CN 4-Pyrimidinamine, 5-bromo-N,2-dicyclopropyl-6-(hexahydro-1H-azepin-1-yl)- (CA INDEX NAME)



RN 617717-05-2 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-6-(hexahydro-1H-azepin-1-yl)- (CA INDEX NAME)



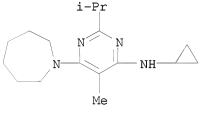
RN 617717-06-3 CAPLUS
CN 4,5-Pyrimidinediamine, N4,2-dicyclopropyl-6-(hexahydro-1H-azepin-1-yl)-
(CA INDEX NAME)



RN 617717-08-5 CAPLUS
CN 4-Pyrimidinamine, N-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl-2-(1-methylethyl)-, (2Z)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

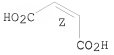
CRN 617717-07-4
CMF C17 H28 N4



CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.

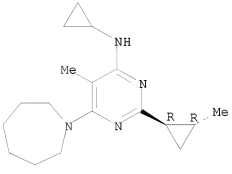


RN 617717-10-9 CAPLUS
CN 4-Pyrimidinamine, N-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl-2-[(1R,2R)-2-methylcyclopropyl]-, rel-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 617717-09-6
CMF C18 H28 N4

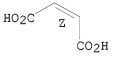
Relative stereochemistry.



CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.

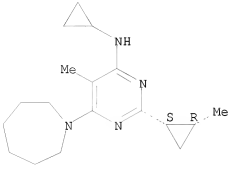


RN 617717-12-1 CAPLUS
CN 4-Pyrimidinamine, N-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl-2-[(1R,2S)-2-methylcyclopropyl]-, rel-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 617717-11-0
CMF C18 H28 N4

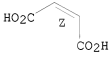
Relative stereochemistry.



CM 2

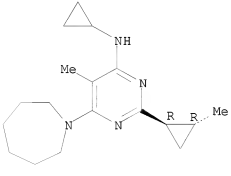
CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.



RN 617717-13-2 CAPLUS
CN 4-Pyrimidinamine, N-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl-2-[(1R,2R)-2-methylcyclopropyl]-, rel-(-)- (CA INDEX NAME)

Rotation (-). Absolute stereochemistry unknown.

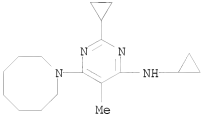


RN 617717-20-1 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-6-(hexahydro-1(2H)-azocinyl)-5-methyl-, (2Z)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

CRN 617717-19-8

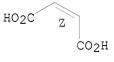
CMF C18 H28 N4



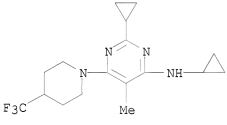
CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.



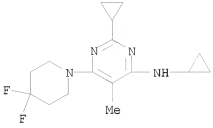
RN 617717-27-8 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-5-methyl-6-[4-(trifluoromethyl)-1-piperidinyl]- (CA INDEX NAME)



RN 617717-29-0 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-6-(4,4-difluoro-1-piperidinyl)-5-methyl-, (2Z)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

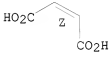
CRN 617717-28-9
CMF C16 H22 F2 N4



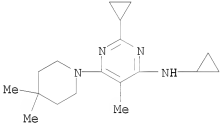
CM 2

CRN 110-16-7
CMF C4 H4 O4

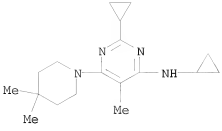
Double bond geometry as shown.



RN 617717-30-3 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-6-(4,4-dimethyl-1-piperidinyl)-5-methyl- (CA INDEX NAME)

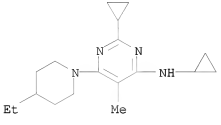


RN 617717-31-4 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-6-(4,4-dimethyl-1-piperidinyl)-5-methyl-, hydrochloride (1:1) (CA INDEX NAME)

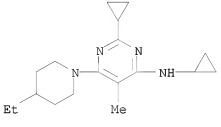


● HCl

RN 617717-39-2 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-6-(4-ethyl-1-piperidinyl)-5-methyl-
(CA INDEX NAME)



RN 617717-40-5 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-6-(4-ethyl-1-piperidinyl)-5-methyl-,
hydrochloride (1:1) (CA INDEX NAME)



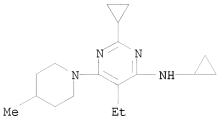
● HCl

RN 617717-49-4 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-5-ethyl-6-(4-methyl-1-piperidinyl)-,
(2Z)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

CRN 617717-48-3

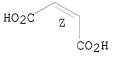
CMF C18 H28 N4



CM 2

CRN 110-16-7
CMF C4 H4 O4

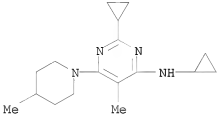
Double bond geometry as shown.



RN 617717-51-8 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-5-methyl-6-(4-methyl-1-piperidinyl)-, (2Z)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

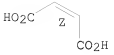
CRN 617717-50-7
CMF C17 H26 N4



CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.

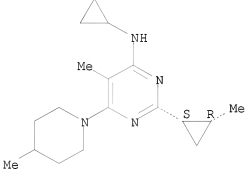


RN 617717-57-4 CAPLUS
CN 4-Pyrimidinamine, N-cyclopropyl-5-methyl-2-[(1R,2S)-2-methylcyclopropyl]-6-(4-methyl-1-piperidinyl)-, rel-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 617717-56-3
CMF C18 H28 N4

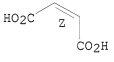
Relative stereochemistry.



CM 2

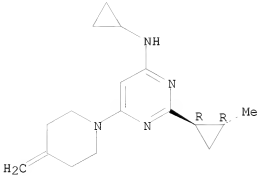
CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.



RN 617717-65-4 CAPLUS
CN 4-Pyrimidinamine, N-cyclopropyl-2-[(1R,2R)-2-methylcyclopropyl]-6-(4-methylene-1-piperidinyl)-, hydrochloride (1:1), rel- (CA INDEX NAME)

Relative stereochemistry.

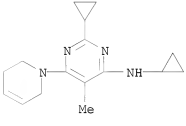


● HCl

RN 617717-75-6 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-6-(3,6-dihydro-1(2H)-pyridinyl)-5-methyl-, (2Z)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

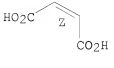
CRN 617717-74-5
CMF C16 H22 N4



CM 2

CRN 110-16-7
CMF C4 H4 O4

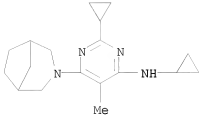
Double bond geometry as shown.



RN 617717-79-0 CAPLUS
CN 4-Pyrimidinamine, 6-(3-azabicyclo[3.2.1]oct-3-yl)-N,2-dicyclopropyl-5-methyl-, (2Z)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

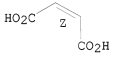
CRN 617717-78-9
CMF C18 H26 N4



CM 2

CRN 110-16-7
CMF C4 H4 O4

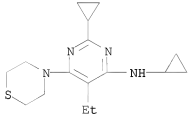
Double bond geometry as shown.



RN 617717-85-8 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-5-ethyl-6-(4-thiomorpholinyl)-, (2Z)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

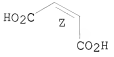
CRN 617717-84-7
CMF C16 H24 N4 S



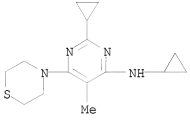
CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.



RN 617717-86-9 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-5-methyl-6-(4-thiomorpholinyl)-, hydrochloride (1:1) (CA INDEX NAME)

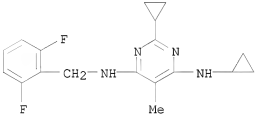


● HCl

RN 617718-04-4 CAPLUS
CN 4,6-Pyrimidinediamine, N,2-dicyclopropyl-N'-[(2,6-difluorophenyl)methyl]-5-methyl-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

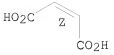
CRN 617718-03-3
CMF C18 H20 F2 N4



CM 2

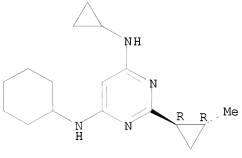
CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.



RN 617718-25-9 CAPLUS
CN 4,6-Pyrimidinediamine, N4-cyclohexyl-N6-cyclopropyl-2-[(1R,2R)-2-methylcyclopropyl]-, rel-(-)- (CA INDEX NAME)

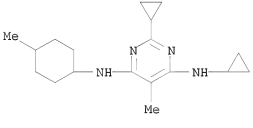
Rotation (-). Absolute stereochemistry unknown.



RN 617718-27-1 CAPLUS
CN 4,6-Pyrimidinediamine, N,2-dicyclopropyl-5-methyl-N'-(4-methylcyclohexyl)-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

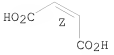
CRN 617718-26-0
CMF C18 H28 N4



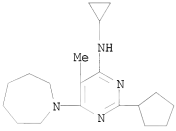
CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.



RN 617718-39-5 CAPLUS
CN 4-Pyrimidinamine, 2-cyclopentyl-N-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl-, hydrochloride (1:1) (CA INDEX NAME)

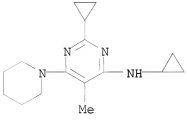


● HCl

RN 617718-62-4 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-5-methyl-6-(1-piperidinyl)-, (2Z)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

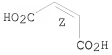
CRN 617718-61-3
CMF C16 H24 N4



CM 2

CRN 110-16-7
CMF C4 H4 O4

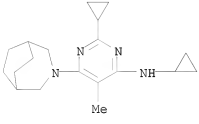
Double bond geometry as shown.



RN 617718-64-6 CAPLUS
CN 4-Pyrimidinamine, 6-(3-azabicyclo[3.2.2]non-3-yl)-N,2-dicyclopropyl-5-methyl-, (2Z)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

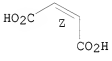
CRN 617718-63-5
CMF C19 H28 N4



CM 2

CRN 110-16-7
CMF C4 H4 O4

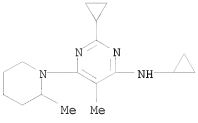
Double bond geometry as shown.



RN 617718-66-8 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-5-methyl-6-(2-methyl-1-piperidinyl)-, (2E)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

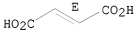
CRN 617718-65-7
CMF C17 H26 N4



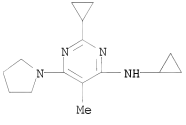
CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.



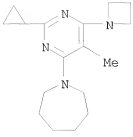
RN 617718-69-1 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-5-methyl-6-(1-pyrrolidinyl)- (CA INDEX NAME)



RN 617718-75-9 CAPLUS
CN 1H-Azepine, 1-[6-(1-azetidinyl)-2-cyclopropyl-5-methyl-4-pyrimidinyl]hexahydro-, (2Z)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

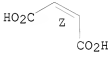
CRN 617718-74-8
CMF C17 H26 N4



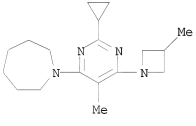
CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.



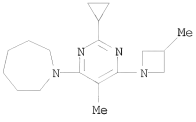
RN 617718-76-0 CAPLUS
CN 1H-Azepine, 1-[2-cyclopropyl-5-methyl-6-(3-methyl-1-azetidinyl)-4-pyrimidinyl]hexahydro- (CA INDEX NAME)



RN 617718-77-1 CAPLUS
CN 1H-Azepine, 1-[2-cyclopropyl-5-methyl-6-(3-methyl-1-azetidinyl)-4-pyrimidinyl]hexahydro-, (2E)-2-butenedioate (2:3) (CA INDEX NAME)

CM 1

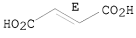
CRN 617718-76-0
CMF C18 H28 N4



CM 2

CRN 110-17-8
CMF C4 H4 O4

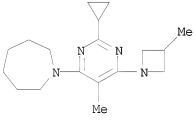
Double bond geometry as shown.



RN 617718-79-3 CAPLUS
CN 1H-Azepine, 1-[2-cyclopropyl-5-methyl-6-(3-methyl-1-azetidinyl)-4-pyrimidinyl]hexahydro-, (2E)-2-butenedioate (1:2) (CA INDEX NAME)

CM 1

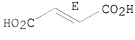
CRN 617718-76-0
CMF C18 H28 N4



CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.

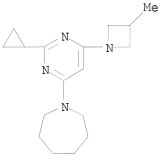


RN 617718-86-2 CAPLUS
CN 1H-Azepine, 1-[2-cyclopropyl-6-(3-methyl-1-azetidinyl)-4-

pyrimidinyl]hexahydro-, (2E)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

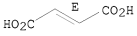
CRN 617718-85-1
CMF C17 H26 N4



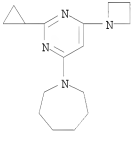
CM 2

CRN 110-17-8
CMF C4 H4 O4

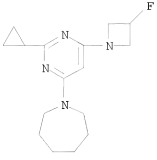
Double bond geometry as shown.



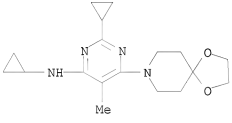
RN 617718-87-3 CAPLUS
CN 1H-Azepine, 1-[6-(1-azetidinyl)-2-cyclopropyl-4-pyrimidinyl]hexahydro- (CA INDEX NAME)



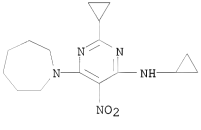
RN 617718-89-5 CAPLUS
CN 1H-Azepine, 1-[2-cyclopropyl-6-(3-fluoro-1-azetidinyl)-4-pyrimidinyl]hexahydro- (CA INDEX NAME)



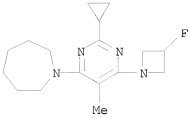
IT 617718-31-7P 617718-93-1P 617719-14-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of aminopyrimidines with muscarinic M3 antagonist and PDE IV inhibiting activity)
RN 617718-31-7 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-6-(1,4-dioxa-8-azaspiro[4.5]dec-8-yl)-5-methyl- (CA INDEX NAME)



RN 617718-93-1 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-nitro- (CA INDEX NAME)



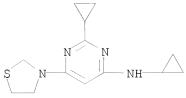
RN 617719-14-9 CAPLUS
CN 1H-Azepine, 1-[2-cyclopropyl-6-(3-fluoro-1-azetidinyl)-5-methyl-4-pyrimidinyl]hexahydro- (CA INDEX NAME)



IT 617716-87-7P 617716-88-8P 617716-99-1P
617717-14-3P 617717-16-5P 617717-17-6P
617717-18-7P 617717-21-2P 617717-22-3P
617717-24-5P 617717-26-7P 617717-32-5P
617717-34-7P 617717-35-8P 617717-36-9P
617717-38-1P 617717-41-6P 617717-42-7P
617717-43-8P 617717-44-9P 617717-45-0P
617717-46-1P 617717-53-0P 617717-55-2P
617717-58-5P 617717-59-6P 617717-60-9P
617717-61-0P 617717-62-1P 617717-63-2P
617717-64-3P 617717-66-5P 617717-67-6P
617717-69-8P 617717-71-2P 617717-73-4P
617717-76-7P 617717-77-8P 617717-81-4P
617717-83-6P 617717-87-0P 617717-88-1P
617717-89-2P 617717-91-6P 617717-92-7P
617717-93-8P 617717-94-9P 617717-95-0P
617717-97-2P 617717-99-4P 617718-00-0P
617718-02-2P 617718-06-6P 617718-07-7P
617718-09-9P 617718-11-3P 617718-13-5P
617718-15-7P 617718-17-9P 617718-19-1P
617718-21-5P 617718-23-7P 617718-24-8P
617718-26-0P 617718-28-2P 617718-30-6P
617718-33-9P 617718-35-1P 617718-37-3P
617718-38-4P 617718-57-7P 617718-59-9P
617718-60-2P 617718-67-9P 617718-68-0P
617718-71-5P 617718-72-6P 617718-73-7P
617718-81-7P 617718-84-0P 617718-88-4P
617718-90-8P 617718-92-0P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of aminopyrimidines with muscarinic M3 antagonist and PDE IV inhibiting activity)

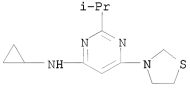
RN 617716-87-7 CAPLUS

CN 4-Pyrimidinamine, N,2-dicyclopropyl-6-(3-thiazolidinyl)-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

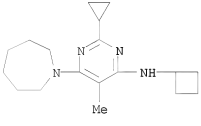
RN 617716-88-8 CAPLUS
CN 4-Pyrimidinamine, N-cyclopropyl-2-(1-methylethyl)-6-(3-thiazolidinyl)-
(CA INDEX NAME)



RN 617716-99-1 CAPLUS
CN 4-Pyrimidinamine, N-cyclobutyl-2-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-
5-methyl-, (2Z)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

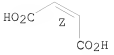
CRN 617716-98-0
CMF C18 H28 N4



CM 2

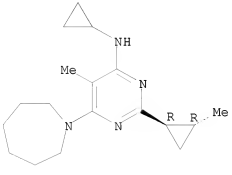
CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.



RN 617717-14-3 CAPLUS
CN 4-Pyrimidinamine, N-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl-2-[(1R,2R)-2-methylcyclopropyl]-, rel-(+)- (CA INDEX NAME)

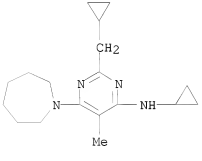
Rotation (+). Absolute stereochemistry unknown.



RN 617717-16-5 CAPLUS
CN 4-Pyrimidinamine, N-cyclopropyl-2-(cyclopropylmethyl)-6-(hexahydro-1H-azepin-1-yl)-5-methyl-, (2Z)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

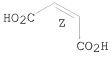
CRN 617717-15-4
CMF C18 H28 N4



CM 2

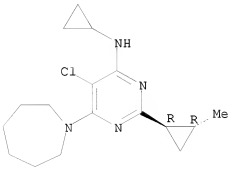
CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.



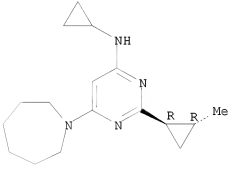
RN 617717-17-6 CAPLUS
CN 4-Pyrimidinamine, 5-chloro-N-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-2-[(1R,2R)-2-methylcyclopropyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.



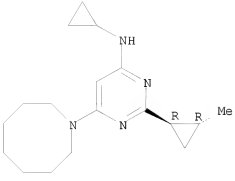
RN 617717-18-7 CAPLUS
CN 4-Pyrimidinamine, N-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-2-[(1R,2R)-2-methylcyclopropyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.

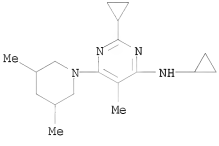


RN 617717-21-2 CAPLUS
CN 4-Pyrimidinamine, N-cyclopropyl-6-(hexahydro-1(2H)-azocinyl)-2-[(1R,2R)-2-methylcyclopropyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.



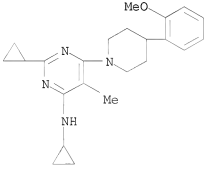
RN 617717-22-3 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-6-(3,5-dimethyl-1-piperidinyl)-5-methyl- (CA INDEX NAME)



RN 617717-24-5 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-6-[4-(2-methoxyphenyl)-1-piperidinyl]-5-methyl-, (2Z)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

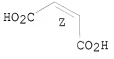
CRN 617717-23-4
CMF C23 H30 N4 O



CM 2

CRN 110-16-7
CMF C4 H4 O4

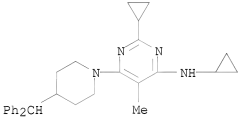
Double bond geometry as shown.



RN 617717-26-7 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-6-[4-(diphenylmethyl)-1-piperidinyl]-5-methyl-, (2Z)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

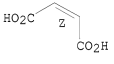
CRN 617717-25-6
CMF C29 H34 N4



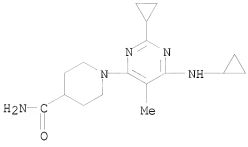
CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.



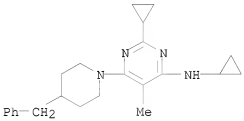
RN 617717-32-5 CAPLUS
CN 4-Piperidinecarboxamide, 1-[2-cyclopropyl-6-(cyclopropylamino)-5-methyl-4-pyrimidinyl]- (CA INDEX NAME)



RN 617717-34-7 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-5-methyl-6-[4-(phenylmethyl)-1-piperidinyl]-, (2Z)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

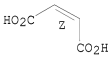
CRN 617717-33-6
CMF C23 H30 N4



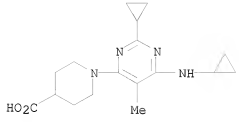
CM 2

CRN 110-16-7
CMF C4 H4 O4

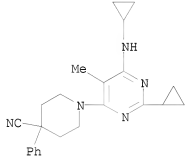
Double bond geometry as shown.



RN 617717-35-8 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[2-cyclopropyl-6-(cyclopropylamino)-5-methyl-4-pyrimidinyl]- (CA INDEX NAME)



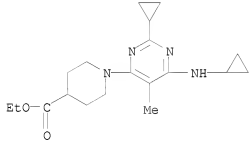
RN 617717-36-9 CAPLUS
CN 4-Piperidinecarbonitrile, 1-[2-cyclopropyl-6-(cyclopropylamino)-5-methyl-4-pyrimidinyl]-4-phenyl- (CA INDEX NAME)



RN 617717-38-1 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[2-cyclopropyl-6-(cyclopropylamino)-5-methyl-4-pyrimidinyl]-, ethyl ester, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

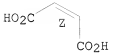
CRN 617717-37-0
CMF C19 H28 N4 O2



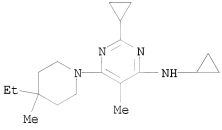
CM 2

CRN 110-16-7
CMF C4 H4 O4

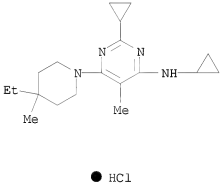
Double bond geometry as shown.



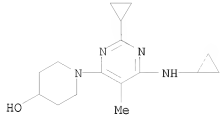
RN 617717-41-6 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-6-(4-ethyl-4-methyl-1-piperidinyl)-5-methyl- (CA INDEX NAME)



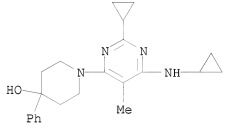
RN 617717-42-7 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-6-(4-ethyl-4-methyl-1-piperidinyl)-5-methyl-, hydrochloride (1:1) (CA INDEX NAME)



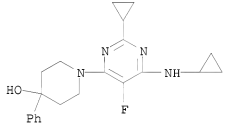
RN 617717-43-8 CAPLUS
CN 4-Piperidinol, 1-[2-cyclopropyl-6-(cyclopropylamino)-5-methyl-4-pyrimidinyl]- (CA INDEX NAME)



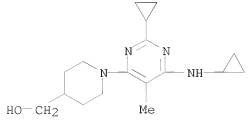
RN 617717-44-9 CAPLUS
CN 4-Piperidinol, 1-[2-cyclopropyl-6-(cyclopropylamino)-5-methyl-4-pyrimidinyl]-4-phenyl- (CA INDEX NAME)



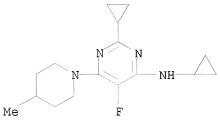
RN 617717-45-0 CAPLUS
CN 4-Piperidinol, 1-[2-cyclopropyl-6-(cyclopropylamino)-5-fluoro-4-pyrimidinyl]-4-phenyl- (CA INDEX NAME)



RN 617717-46-1 CAPLUS
CN 4-Piperidinemethanol, 1-[2-cyclopropyl-6-(cyclopropylamino)-5-methyl-4-pyrimidinyl]- (CA INDEX NAME)

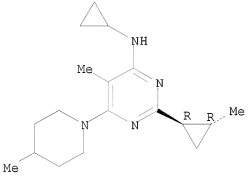


RN 617717-53-0 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-5-fluoro-6-(4-methyl-1-piperidinyl)-
(CA INDEX NAME)



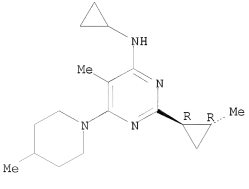
RN 617717-55-2 CAPLUS
CN 4-Pyrimidinamine, N-cyclopropyl-5-methyl-2-[(1R,2R)-2-methylcyclopropyl]-6-
(4-methyl-1-piperidinyl)-, rel- (CA INDEX NAME)

Relative stereochemistry.



RN 617717-58-5 CAPLUS
CN 4-Pyrimidinamine, N-cyclopropyl-5-methyl-2-[(1R,2R)-2-methylcyclopropyl]-6-
(4-methyl-1-piperidinyl)-, rel-(+)- (CA INDEX NAME)

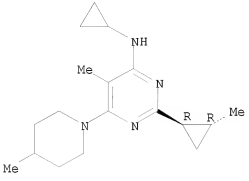
Rotation (+). Absolute stereochemistry unknown.



RN 617717-59-6 CAPLUS

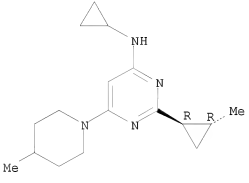
CN 4-Pyrimidinamine, N-cyclopropyl-5-methyl-2-[(1R,2R)-2-methylcyclopropyl]-6-(4-methyl-1-piperidinyl)-, rel-(-)- (CA INDEX NAME)

Rotation (-). Absolute stereochemistry unknown.



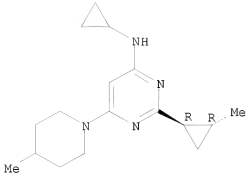
RN 617717-60-9 CAPLUS
CN 4-Pyrimidinamine, N-cyclopropyl-2-[(1R,2R)-2-methylcyclopropyl]-6-(4-methyl-1-piperidinyl)-, rel- (CA INDEX NAME)

Relative stereochemistry.



RN 617717-61-0 CAPLUS
CN 4-Pyrimidinamine, N-cyclopropyl-2-[(1R,2R)-2-methylcyclopropyl]-6-(4-methyl-1-piperidinyl)-, hydrochloride (1:1), rel- (CA INDEX NAME)

Relative stereochemistry.



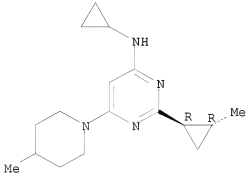
● HCl

RN 617717-62-1 CAPLUS
CN 4-Pyrimidinamine, N-cyclopropyl-2-[(1R,2R)-2-methylcyclopropyl]-6-(4-methyl-1-piperidinyl)-, rel-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 617717-60-9
CMF C17 H26 N4

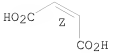
Relative stereochemistry.



CM 2

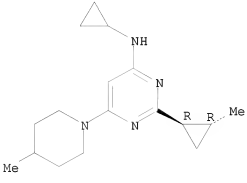
CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.



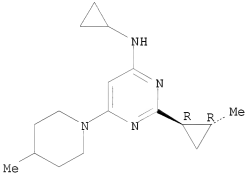
RN 617717-63-2 CAPLUS
CN 4-Pyrimidinamine, N-cyclopropyl-2-[(1R,2R)-2-methylcyclopropyl]-6-(4-methyl-1-piperidinyl)-, rel-(+)- (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.

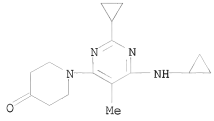


RN 617717-64-3 CAPLUS
CN 4-Pyrimidinamine, N-cyclopropyl-2-[(1R,2R)-2-methylcyclopropyl]-6-(4-methyl-1-piperidinyl)-, rel-(-)- (CA INDEX NAME)

Rotation (-). Absolute stereochemistry unknown.

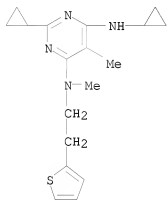


RN 617717-66-5 CAPLUS
CN 4-Piperidinone, 1-[2-cyclopropyl-6-(cyclopropylamino)-5-methyl-4-pyrimidinyl]-, hydrate (1:1) (CA INDEX NAME)



● H_2O

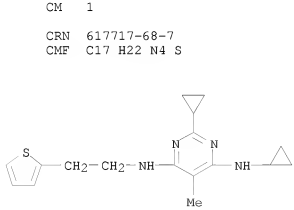
RN 617717-67-6 CAPLUS
CN 4,6-Pyrimidinediamine, N6,2-dicyclopropyl-N4,5-dimethyl-N4-[2-(2-thienyl)ethyl]- (CA INDEX NAME)



RN 617717-69-8 CAPLUS
CN 4,6-Pyrimidinediamine, N,2-dicyclopropyl-5-methyl-N'-[2-(2-thienyl)ethyl]-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

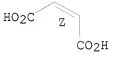
CRN 617717-68-7
CMF C17 H22 N4 S



CM 2

CRN 110-16-7
CMF C4 H4 O4

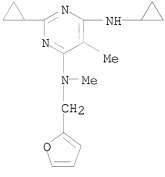
Double bond geometry as shown.



RN 617717-71-2 CAPLUS
CN 4,6-Pyrimidinediamine, N',2-dicyclopropyl-N-(2-furanylmethyl)-N,5-dimethyl-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

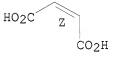
CRN 617717-70-1
CMF C17 H22 N4 O



CM 2

CRN 110-16-7
CMF C4 H4 O4

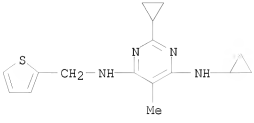
Double bond geometry as shown.



RN 617717-73-4 CAPLUS
CN 4,6-Pyrimidinediamine, N,2-dicyclopropyl-5-methyl-N'-(2-thienylmethyl)-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

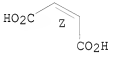
CRN 617717-72-3
CMF C16 H20 N4 S



CM 2

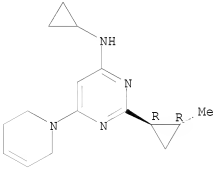
CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.



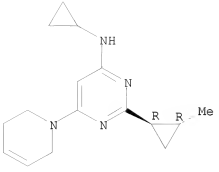
RN 617717-76-7 CAPLUS
CN 4-Pyrimidinamine, N-cyclopropyl-6-(3,6-dihydro-1(2H)-pyridinyl)-2-[(1R,2R)-2-methylcyclopropyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.



RN 617717-77-8 CAPLUS
CN 4-Pyrimidinamine, N-cyclopropyl-6-(3,6-dihydro-1(2H)-pyridinyl)-2-[(1R,2R)-2-methylcyclopropyl]-, hydrochloride (1:1), rel- (CA INDEX NAME)

Relative stereochemistry.

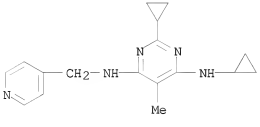


● HCl

RN 617717-81-4 CAPLUS
CN 4,6-Pyrimidinediamine, N,2-dicyclopropyl-5-methyl-N'-(4-pyridinylmethyl)-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

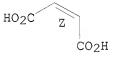
CRN 617717-80-3
CMF C17 H21 N5



CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.

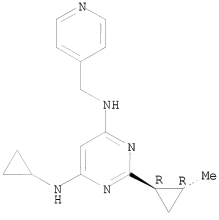


RN 617717-83-6 CAPLUS
CN 4,6-Pyrimidinediamine, N-cyclopropyl-2-[(1R,2R)-2-methylcyclopropyl]-N'-(4-pyridinylmethyl)-, rel-, (2Z)-2-butenedioate (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 617717-82-5
CMF C17 H21 N5

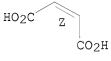
Relative stereochemistry.



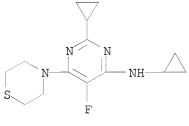
CM 2

CRN 110-16-7
CMF C4 H4 O4

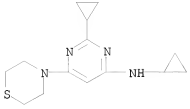
Double bond geometry as shown.



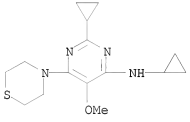
RN 617717-87-0 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-5-fluoro-6-(4-thiomorpholinyl)- (CA INDEX NAME)



RN 617717-88-1 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-6-(4-thiomorpholinyl)- (CA INDEX NAME)



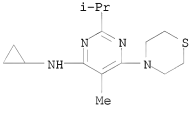
RN 617717-89-2 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-5-methoxy-6-(4-thiomorpholinyl)- (CA INDEX NAME)



RN 617717-91-6 CAPLUS
CN 4-Pyrimidinamine, N-cyclopropyl-5-methyl-2-(1-methylethyl)-6-(4-thiomorpholinyl)-, (2Z)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

CRN 617717-90-5
CMF C15 H24 N4 S



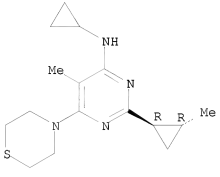
CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.

RN 617717-92-7 CAPLUS
CN 4-Pyrimidinamine, N-cyclopropyl-5-methyl-2-[(1R,2R)-2-methylcyclopropyl]-6-(4-thiomorpholinyl)-, hydrochloride (1:1), rel-(+)- (CA INDEX NAME)

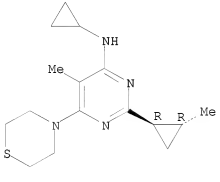
Rotation (+). Absolute stereochemistry unknown.



● HCl

RN 617717-93-8 CAPLUS
CN 4-Pyrimidinamine, N-cyclopropyl-5-methyl-2-[(1R,2R)-2-methylcyclopropyl]-6-(4-thiomorpholinyl)-, hydrochloride (1:1), rel-(-)- (CA INDEX NAME)

Rotation (-). Absolute stereochemistry unknown.

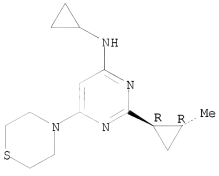


● HCl

RN 617717-94-9 CAPLUS
CN 4-Pyrimidinamine, N-cyclopropyl-2-[(1R,2R)-2-methylcyclopropyl]-6-(4-

thiomorpholinyl)-, hydrochloride (1:1), rel-(+)- (CA INDEX NAME)

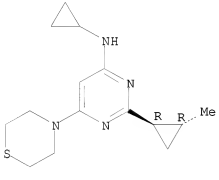
Rotation (+). Absolute stereochemistry unknown.



● HCl

RN 617717-95-0 CAPLUS
CN 4-Pyrimidinamine, N-cyclopropyl-2-[(1R,2R)-2-methylcyclopropyl]-6-(4-thiomorpholinyl)-, hydrochloride (1:1), rel-(-)- (CA INDEX NAME)

Rotation (-). Absolute stereochemistry unknown.

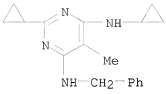


● HCl

RN 617717-97-2 CAPLUS
CN 4,6-Pyrimidinediamine, N,2-dicyclopropyl-5-methyl-N'-(phenylmethyl)-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

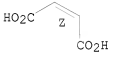
CRN 617717-96-1
CMF C18 H22 N4



CM 2

CRN 110-16-7
CMF C4 H4 O4

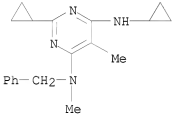
Double bond geometry as shown.



RN 617717-99-4 CAPLUS
CN 4,6-Pyrimidinediamine, N',2-dicyclopropyl-N,5-dimethyl-N-(phenylmethyl)-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

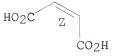
CRN 617717-98-3
CMF C19 H24 N4



CM 2

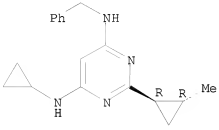
CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.



RN 617718-00-0 CAPLUS
CN 4,6-Pyrimidinediamine, N4-cyclopropyl-2-[(1R,2R)-2-methylcyclopropyl]-N6-(phenylmethyl)-, hydrobromide (1:1), rel- (CA INDEX NAME)

Relative stereochemistry.

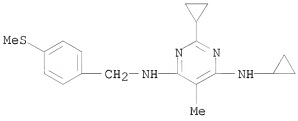


● HBr

RN 617718-02-2 CAPLUS
CN 4,6-Pyrimidinediamine, N,2-dicyclopropyl-5-methyl-N'-[[4-(methylthio)phenyl]methyl]-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

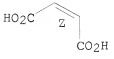
CRN 617718-01-1
CMF C19 H24 N4 S



CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.

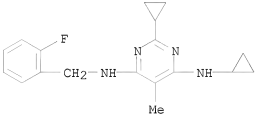


RN 617718-06-6 CAPLUS

CN 4,6-Pyrimidinediamine, N,2-dicyclopropyl-N'-[(2-fluorophenyl)methyl]-5-methyl-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

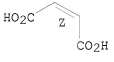
CRN 617718-05-5
CMF C18 H21 F N4



CM 2

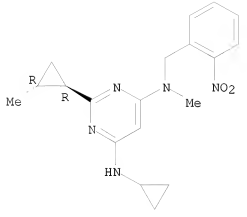
CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.



RN 617718-07-7 CAPLUS
CN 4,6-Pyrimidinediamine, N6-cyclopropyl-N4-methyl-2-[(1R,2R)-2-methylcyclopropyl]-N4-[(2-nitrophenyl)methyl]-, hydrochloride (1:1), rel- (CA INDEX NAME)

Relative stereochemistry.

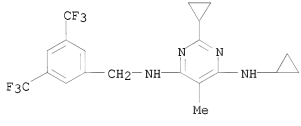


● HCl

RN 617718-09-9 CAPLUS
CN 4,6-Pyrimidinediamine, N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-N',2-dicyclopropyl-5-methyl-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

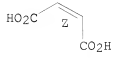
CRN 617718-08-8
CMF C20 H20 F6 N4



CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.

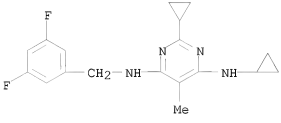


RN 617718-11-3 CAPLUS

CN 4,6-Pyrimidinediamine, N,2-dicyclopropyl-N'-[(3,5-difluorophenyl)methyl]-5-methyl-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

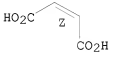
CRN 617718-10-2
CMF C18 H20 F2 N4



CM 2

CRN 110-16-7
CMF C4 H4 O4

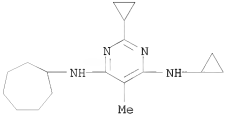
Double bond geometry as shown.



RN 617718-13-5 CAPLUS
CN 4,6-Pyrimidinediamine, N-cycloheptyl-N',2-dicyclopropyl-5-methyl-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 617718-12-4
CMF C18 H28 N4

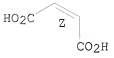


CM 2

CRN 110-16-7

CMF C4 H4 O4

Double bond geometry as shown.

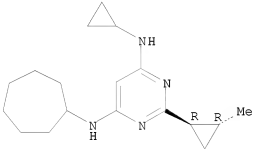


RN 617718-15-7 CAPLUS
CN 4,6-Pyrimidinediamine, N-cycloheptyl-N'-cyclopropyl-2-[(1R,2R)-2-methylcyclopropyl]-, rel-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 617718-14-6
CMF C18 H28 N4

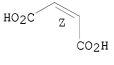
Relative stereochemistry.



CM 2

CRN 110-16-7
CMF C4 H4 O4

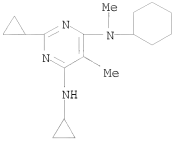
Double bond geometry as shown.



RN 617718-17-9 CAPLUS
CN 4,6-Pyrimidinediamine, N-cyclohexyl-N',2-dicyclopropyl-N,5-dimethyl-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

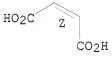
CRN 617718-16-8
CMF C18 H28 N4



CM 2

CRN 110-16-7
CMF C4 H4 O4

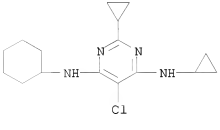
Double bond geometry as shown.



RN 617718-19-1 CAPLUS
CN 4,6-Pyrimidinediamine, 5-chloro-N-cyclohexyl-N',2-dicyclopropyl-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

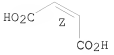
CRN 617718-18-0
CMF C16 H23 Cl N4



CM 2

CRN 110-16-7
CMF C4 H4 O4

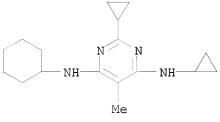
Double bond geometry as shown.



RN 617718-21-5 CAPLUS
CN 4,6-Pyrimidinediamine, N-cyclohexyl-N',2-dicyclopropyl-5-methyl-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

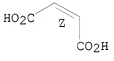
CRN 617718-20-4
CMF C17 H26 N4



CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.

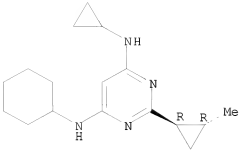


RN 617718-23-7 CAPLUS
CN 4,6-Pyrimidinediamine, N-cyclohexyl-N'-cyclopropyl-2-[(1R,2R)-2-methylcyclopropyl]-, rel-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 617718-22-6
CMF C17 H26 N4

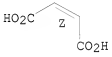
Relative stereochemistry.



CM 2

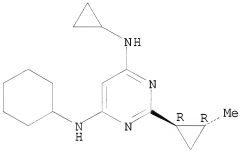
CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.

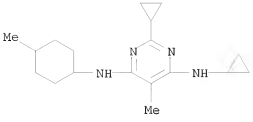


RN 617718-24-8 CAPLUS
CN 4,6-Pyrimidinediamine, N4-cyclohexyl-N6-cyclopropyl-2-[(1R,2R)-2-methylcyclopropyl]-, rel-(+)- (CA INDEX NAME)

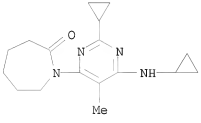
Rotation (+). Absolute stereochemistry unknown.



RN 617718-26-0 CAPLUS
CN 4,6-Pyrimidinediamine, N4,2-dicyclopropyl-5-methyl-N6-(4-methylcyclohexyl)- (CA INDEX NAME)



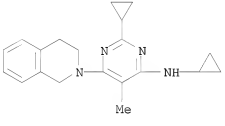
RN 617718-28-2 CAPLUS
CN 2H-Azepin-2-one, 1-[2-cyclopropyl-6-(cyclopropylamino)-5-methyl-4-pyrimidinyl]hexahydro- (CA INDEX NAME)



RN 617718-30-6 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-6-(3,4-dihydro-2(1H)-isoquinolinyl)-5-methyl-, (2Z)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

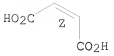
CRN 617718-29-3
CMF C20 H24 N4



CM 2

CRN 110-16-7
CMF C4 H4 O4

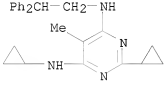
Double bond geometry as shown.



RN 617718-33-9 CAPLUS
CN 4,6-Pyrimidinediamine, N,2-dicyclopropyl-N'-(2,2-diphenylethyl)-5-methyl-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

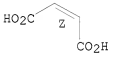
CRN 617718-32-8
CMF C25 H28 N4



CM 2

CRN 110-16-7
CMF C4 H4 O4

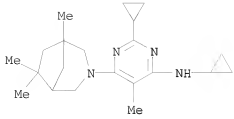
Double bond geometry as shown.



RN 617718-35-1 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-5-methyl-6-(1,6,6-trimethyl-3-azabicyclo[3.2.1]oct-3-yl)-, (2Z)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

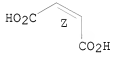
CRN 617718-34-0
CMF C21 H32 N4



CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.

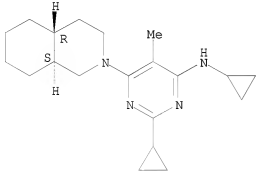


RN 617718-37-3 CAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-5-methyl-6-[(4aR,8aS)-octahydro-2(1H)-isoquinolinyl]-, rel-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 617718-36-2
CMF C20 H30 N4

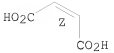
Relative stereochemistry.



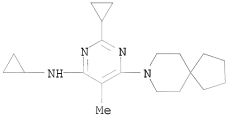
CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.



RN 617718-38-4 CAPLUS
CN 4-Pyrimidinamine, 6-(8-azaspiro[4.5]dec-8-yl)-N,2-dicyclopropyl-5-methyl-, hydrochloride (1:1) (CA INDEX NAME)



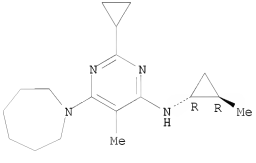
● HCl

RN 617718-57-7 CAPLUS
CN 4-Pyrimidinamine, 2-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl-N-[(1R,2R)-2-methylcyclopropyl]-, rel-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 617718-56-6
CMF C18 H28 N4

Relative stereochemistry.



CM 2

CRN 110-17-8
CMF C4 H4 O4

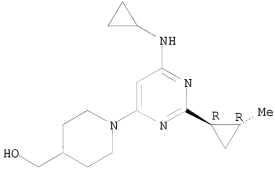
Double bond geometry as shown.

RN 617718-59-9 CAPLUS
CN 4-Piperidinemethanol, 1-[6-(cyclopropylamino)-2-[(1R,2R)-2-methylcyclopropyl]-4-pyrimidinyl]-, rel-, (2Z)-2-butenedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 617718-58-8
CMF C17 H26 N4 O

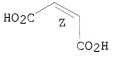
Relative stereochemistry.



CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.

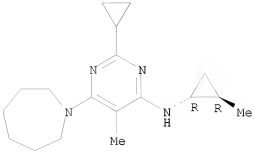


RN 617718-60-2 CAPLUS
CN 4-Pyrimidinamine, 2-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl-N-[(1R,2R)-2-methylcyclopropyl]-, rel-, (2E)-2-butenedioate (2:3) (9CI) (CA INDEX NAME)

CM 1

CRN 617718-56-6
CMF C18 H28 N4

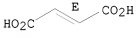
Relative stereochemistry.



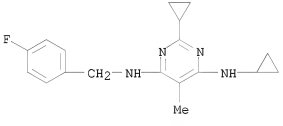
CM 2

CRN 110-17-8
CMF C4 H4 O4

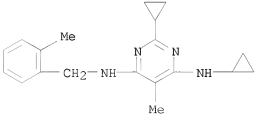
Double bond geometry as shown.



RN 617718-67-9 CAPLUS
CN 4,6-Pyrimidinediamine, N4,2-dicyclopropyl-N6-[(4-fluorophenyl)methyl]-5-methyl- (CA INDEX NAME)



RN 617718-68-0 CAPLUS
CN 4,6-Pyrimidinediamine, N4,2-dicyclopropyl-5-methyl-N6-[(2-methylphenyl)methyl]- (CA INDEX NAME)



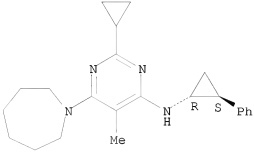
RN 617718-71-5 CAPLUS

CN 4-Pyrimidinamine, 2-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl-N-[(1R,2S)-2-phenylcyclopropyl]-, rel-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 617718-70-4
CMF C23 H30 N4

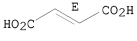
Relative stereochemistry.



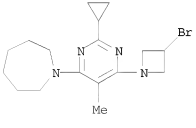
CM 2

CRN 110-17-8
CMF C4 H4 O4

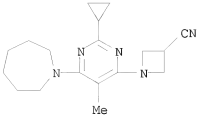
Double bond geometry as shown.



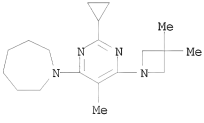
RN 617718-72-6 CAPLUS
CN 1H-Azepine, 1-[6-(3-bromo-1-azetidinyl)-2-cyclopropyl-5-methyl-4-pyrimidinyl]hexahydro- (CA INDEX NAME)



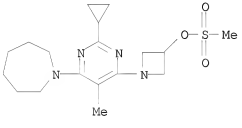
RN 617718-73-7 CAPLUS
CN 3-Azetidinecarbonitrile, 1-[2-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl-4-pyrimidinyl]- (CA INDEX NAME)



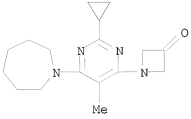
RN 617718-81-7 CAPLUS
CN 1H-Azepine, 1-[2-cyclopropyl-6-(3,3-dimethyl-1-azetidinyl)-5-methyl-4-pyrimidinyl]hexahydro- (CA INDEX NAME)



RN 617718-84-0 CAPLUS
CN 3-Azetidinol, 1-[2-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl-4-pyrimidinyl]-, 3-methanesulfonate (CA INDEX NAME)



RN 617718-88-4 CAPLUS
CN 3-Azetidinone, 1-[2-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl-4-pyrimidinyl]-, hydrate (1:1) (CA INDEX NAME)

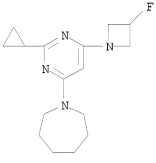


● H_2O

RN 617718-90-8 CAPLUS
CN 1H-Azepine, 1-[2-cyclopropyl-6-(3-fluoro-1-azetidinyl)-4-pyrimidinyl]hexahydro-, (2E)-2-butenedioate (2:3) (CA INDEX NAME)

CM 1

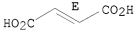
CRN 617718-89-5
CMF C16 H23 F N4



CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.

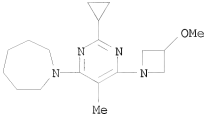


RN 617718-92-0 CAPLUS
CN 1H-Azepine, 1-[2-cyclopropyl-6-(3-methoxy-1-azetidinyl)-5-methyl-4-pyrimidinyl]hexahydro-, (2Z)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

CRN 617718-91-9

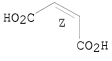
CMF C18 H28 N4 O



CM 2

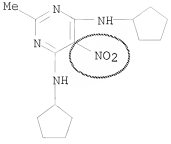
CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.



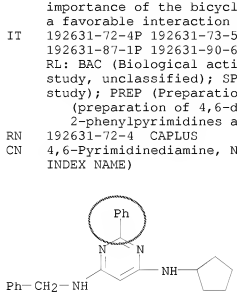
RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2003:775798 CAPLUS
DN 140:192821
TI N,N'-dicyclopentyl-2-methylsulfanyl-5-nitro-pyrimidine-4,6-diamine (GS39783) and structurally related compounds: Novel allosteric enhancers of γ-aminobutyric acidB receptor function
AU Urwyler, Stephan; Pozza, Mario F.; Lingenhoehl, Kurt; Mosbacher, Johannes; Lampert, Christina; Froestl, Wolfgang; Koller, Manuel; Kaupmann, Klemens
CS Novartis Institutes for BioMedical Research, Novartis Pharma AG, Basel, Switz.
SO Journal of Pharmacology and Experimental Therapeutics (2003), 307(1), 322-330
CODEN: JPETAB; ISSN: 0022-3565
PB American Society for Pharmacology and Experimental Therapeutics
DT Journal
LA English
AB N,N'-Dicyclopentyl-2-methylsulfanyl-5-nitro-pyrimidine-4,6-diamine (GS39783) and structurally related compds. are described as novel allosteric enhancers of GABAB receptor function. They potentiate GABA-stimulated guanosine 5'-O-(3-[35S]thio)-triphosphate ([35S]GTPγS) binding to membranes from a GABAB(1b/2)-expressing Chinese hamster ovary cell line at low micromolar concns., but do not stimulate [35S]GTPγS binding by themselves. Similar effects of GS39783 are seen on native GABAB receptors in rat brain membranes. Concentration-response curves with GABA in the presence of different fixed concns. of GS39783 reveal an increase of both the potency and maximal efficacy of GABA at the GABAB(1b/2) heterodimer. In radioligand binding expts., GS39783 reduces the kinetic rate consts. of the association and dissociation of [3H]3-aminopropylphosphinic acid, resulting in a net increase in affinity for the agonist radioligand. In equilibrium binding expts. (displacement of the antagonist ligand [3H]CGP62349), GS39783 increases agonist affinities. Agonist displacement curves are biphasic, probably reflecting the G protein-coupled and uncoupled states of the receptor. The proportion of the high-affinity component is increased by GS39783, suggesting that the G protein coupling of the receptor is also promoted by the pos. modulator. We also show that GS39783 has modulatory effects in cellular assays such as GABAB receptor-mediated activation of inwardly rectifying potassium channels in Xenopus oocytes and Ca2+ signaling in human embryonic kidney 293 cells. In a more physiol. context, GS39783 is shown to suppress paired pulse inhibition in rat hippocampal slices. This effect is reversed by the competitive GABAB receptor antagonist CGP55845A and is produced most likely by enhancing the effect of synaptically released GABA at presynaptic GABAB receptors.
IT 53039-20-6, CGA 38493
RL: PAC (Pharmacological activity); BIOL (Biological study)
(GS39783 and structurally related compds. as novel allosteric enhancers of GABABB receptor function)
RN 53039-20-6 CAPLUS
CN 4,6-Pyrimidinediamine, N,N'-dicyclopentyl-2-methyl-5-nitro- (9CI) (CA INDEX NAME)

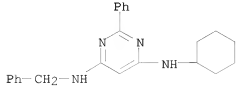


RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1997:407610 CAPLUS
DN 127:121691
OREF 127:23473a,23476a
TI Synthesis of 4,6-disubstituted and 4,5,6-trisubstituted 2-phenylpyrimidines and their affinity towards A1 adenosine receptors
AU Biagi, Giuliana; Giorgi, Irene; Livi, Oreste; Scartoni, Valerio; Lucacchini, Antonio
CS Dip. Scienze Farmaceutiche, Univ. Pisa, Pisa, 56126, Italy
SO Farmaco (1997), 52(1), 61-65
CODEN: FRMCE8; ISSN: 0014-827X
PB Societa Chimica Italiana
DT Journal
LA English
AB The preparation and assay of the title compds., e.g., I (R = cyclohexyl, pentyl), are reported. The results support our hypothesis about the possibility that mols. characterized by great flexibility, such as 2-phenyl-4,5,6-triaminopyrimidines, can better interact with the receptor sites than rigid mols. such as 2,6,9-trisubstituted 8-azaadenines. The relatively low activity shown by pyrimidine derivs. demonstrated the importance of the bicyclic aromatic system in 8-azaadenines and adenines for a favorable interaction with the A1 adenosine receptors.
IT 192631-72-4P 192631-73-5P 192631-86-0P
192631-87-1P 192631-90-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of 4,6-disubstituted and 4,5,6-trisubstituted 2-phenylpyrimidines and their A1 adenosine receptor affinity)
RN 192631-72-4 CAPLUS
CN 4,6-Pyrimidinediamine, N4-cyclopentyl-2-phenyl-N6-(phenylmethyl)- (CA INDEX NAME)

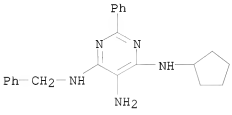


RN 192631-73-5 CAPLUS
CN 4,6-Pyrimidinediamine, N4-cyclohexyl-2-phenyl-N6-(phenylmethyl)- (CA INDEX NAME)



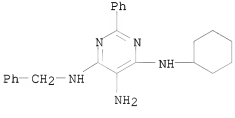
RN 192631-86-0 CAPLUS
CN 4,5,6-Pyrimidinetriamine, N4-cyclopentyl-2-phenyl-N6-(phenylmethyl)-,

monohydrochloride (9CI) (CA INDEX NAME)



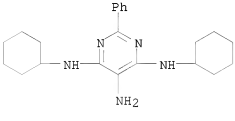
● HCl

RN 192631-87-1 CAPLUS
CN 4,5,6-Pyrimidinetriamine, N4-cyclohexyl-2-phenyl-N6-(phenylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 192631-90-6 CAPLUS
CN 4,5,6-Pyrimidinetriamine, N4,N6-dicyclohexyl-2-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)

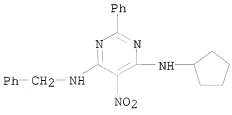


● HCl

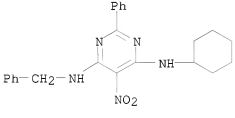
IT 192631-78-0P 192631-79-1P 192631-82-6P
192631-83-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 4,6-disubstituted and 4,5,6-trisubstituted 2-phenylpyrimidines and their A1 adenosine receptor affinity)

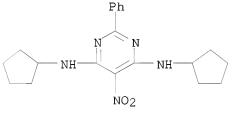
RN 192631-78-0 CAPLUS
CN 4,6-Pyrimidinediamine, N4-cyclopentyl-5-nitro-2-phenyl-N6-(phenylmethyl)- (CA INDEX NAME)



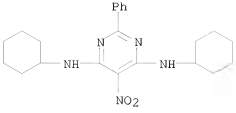
RN 192631-79-1 CAPLUS
CN 4,6-Pyrimidinediamine, N4-cyclohexyl-5-nitro-2-phenyl-N6-(phenylmethyl)- (CA INDEX NAME)



RN 192631-82-6 CAPLUS
CN 4,6-Pyrimidinediamine, N4,N6-dicyclopentyl-5-nitro-2-phenyl- (CA INDEX NAME)



RN 192631-83-7 CAPLUS
CN 4,6-Pyrimidinediamine, N4,N6-dicyclohexyl-5-nitro-2-phenyl- (CA INDEX NAME)


Ph
N
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NH
NH
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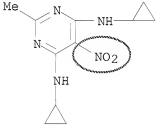
L4 ANSWER 11 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1978:615426 CAPLUS
DN 89:215426
OREF 89:33481a,33484a
TI Nitropyrimidine derivatives
IN Fischer, Hanspeter
PA Ciba-Geigy A.-G., Switz.
SO Pat. Specif. (Aust.), 41 pp.
CODEN: ALXXAP
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	AU 492126	B	19780303	AU 1974-68921	19740514
PRAI	AU 1974-68921		19740514		

AB Eighty nitropyrimidines I (R1 = C1-6 alkyl, C2-5 alkenyl, C3-6 un- or Me- or Et-substituted cycloalkyl, alkoxy-, cyano-, or hydroxyalkyl; R2, R3 = H, C1-4 alkyl; R4 alkyl, C3-4 alkenyl, C3-6 un- or Me- or Et-substituted cycloalkyl; R5 = H, alkyl, haloalkyl, alkoxy, alkyl- or dialkylamino) and their acid addition salts, useful as herbicides and plant growth inhibitors (extensive data tabulated), were prepared by 3 methods. Thus, EtNH2(g) was passed into dichloropyrimidine II (R5 = MeS) in alc. at .apprx.35° and the mixture stirred 2 h at room temperature to give I (R1 = R3 = Et, R2 = R4 = H, R5 = MeS), which was refluxed 20 h with stirring with NaOMe-MeOH to give I (R1 = R3 = Et, R2 = R4 = H, R5 = MeO).

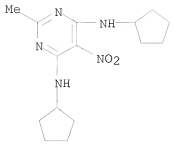
IT 53039-12-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and herbicidal activity of)

RN 53039-12-6 CAPLUS
CN 4,6-Pyrimidinediamine, N,N'-dicyclopropyl-2-methyl-5-nitro- (9CI) (CA INDEX NAME)



IT 53039-20-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 53039-20-6 CAPLUS
CN 4,6-Pyrimidinediamine, N,N'-dicyclopentyl-2-methyl-5-nitro- (9CI) (CA INDEX NAME)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N
NH
N
NO2
NH

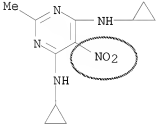
L4 ANSWER 12 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1976:429570 CAPLUS
DN 85:29570
OREF 85:4793a,4796a
TI 5-Nitropyrimidines for inhibiting plant growth
PA Ciba-Geigy A.-G., Switz.
SO Austrian, 20 pp.
CODEN: AUXXAK
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	AT 327605	B	19760210	AT 1974-3729	19740506
	AT 7403729	A	19750415		
PRAI	AT 1974-3729	A	19740506		

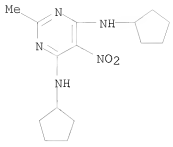
AB The title compds. I(R1 = C1-6 alkyl, C2-5 alkenyl, cycloalkyl, alkoxyalkyl, hydroxyalkyl, or cyanoalkyl; R2 and R3 = H or C1-4 alkyl; R4 = lower alkyl or cycloalkyl; R5 = H, lower alkoxy, alkyl, haloalkyl, alkylamino, dialkylamino, or halogen) are herbicides and plant-growth regulators. Thus 4 kg I(R1 = R4 = Et; R2 = R3 = H; R5 = iso-Pr) [53038-76-9]/ha controlled Cyperus esculentus without damaging alfalfa. Several syntheses are described.

IT 53039-12-6P 53039-20-6P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as herbicide)

RN 53039-12-6 CAPLUS
CN 4,6-Pyrimidinediamine, N,N'-dicyclopropyl-2-methyl-5-nitro- (9CI) (CA INDEX NAME)



RN 53039-20-6 CAPLUS
CN 4,6-Pyrimidinediamine, N,N'-dicyclopentyl-2-methyl-5-nitro- (9CI) (CA INDEX NAME)


Me
N
NH
N
NO2
NH

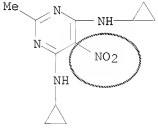
L4 ANSWER 13 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1975:27230 CAPLUS
DN 82:27230
OREF 82:4329a,4332a
TI Nitropyrimidine plant growth regulators [herbicides]
IN Fischer, Hanspeter
PA Ciba-Geigy A.-G.
SO Ger. Offen., 44 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2356644	A1	19740522	DE 1973-2356644	19731113
	CH 574206	A5	19760415	CH 1972-16728	19721116
	US 3948914	A	19760406	US 1973-415209	19731112
	CA 1011960	A1	19770614	CA 1973-185680	19731113
	BE 807321	A1	19740514	BE 1973-137749	19731114
	FR 2206909	A1	19740614	FR 1973-40409	19731114
	NL 7315695	A	19740520	NL 1973-15695	19731115
	ZA 7308750	A	19740731	ZA 1973-8750	19731115
	JP 49081538	A	19740806	JP 1973-128692	19731115
	IT 1001780	B	19760430	IT 1973-31377	19731115
	GB 1448851	A	19760908	GB 1973-53090	19731115
	GB 1448852	A	19760908	GB 1975-8912	19731115
	US 4055411	A	19771025	US 1975-641792	19751218
PRAI	CH 1972-16728	A	19721116		
	US 1973-415209	A3	19731112		

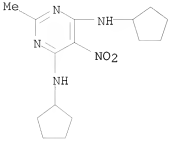
AB 4,6-Dialkylamino-5-nitropyrimidines I (R,R1,R2 and R3 = H, alkyl or alkenyl; R4 = alkyl, CF3, Cl or alkylamino) were especially effective as herbicides. For example, 4,6-bis(ethylamino)-5-nitro-2-isopropylpyrimidine (I, R = R2 = Et, R1 = R3 = H, R4 = iso-Pr) [53038-76-9] 4kg/ha, controlled Cyperus esculentus, Digitaria sanguinalis, Amaranthus, Setaria italica, and Echinochloa crus-galli, with little or no phytotoxicity to culture plants.

IT 53039-12-6 53039-20-6
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses)
(herbicide)

RN 53039-12-6 CAPLUS
CN 4,6-Pyrimidinediamine, N,N'-dicyclopropyl-2-methyl-5-nitro- (9CI) (CA INDEX NAME)



RN 53039-20-6 CAPLUS
CN 4,6-Pyrimidinediamine, N,N'-dicyclopentyl-2-methyl-5-nitro- (9CI) (CA INDEX NAME)



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=> log y
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                      ENTRY     SESSION
FULL ESTIMATED COST                                    71.81      250.84

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                      ENTRY     SESSION
CA SUBSCRIBER PRICE                                   -10.40      -10.40

STN INTERNATIONAL LOGOFF AT 15:33:21 ON 01 AUG 2008
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